CONTACT INTERACTIONS IN QUANTUM MECHANICS: THEORY, MATHEMATICAL ASPECTS AND APPLICATIONS

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CONTACT INTERACTIONS IN QUANTUM MECHANICS: THEORY, MATHEMATICAL ASPECTS AND APPLICATIONS

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Table of Contents

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EDITORIAL
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Editorial: Contact Interactions in Quantum Mechanics–Theory, Mathematical Aspects and Applications

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Keywords: contact interactions, singular potentials, point interactions, self-adjoint extensions of symmetric operators, regularization and renormalization methods, theory of distributions, solvable models in Quantum Mechanics

Editorial on the Research Topic

Contact Interactions in Quantum Mechanics: Theory, Mathematical Aspects and Applications

Contact interactions refer to a broad range of interactions usually described by potentials with support on a set of dimension lower than the dimension of the ambient space. Typical examples are point potentials given by Dirac deltas, finite or infinite combinations of Dirac deltas or its derivatives, and other types of interactions supported on curves, surfaces, and manifolds. In the last thirty years contact interactions in quantum mechanics have attracted a growing interest, since they provide solvable or quasi solvable models which are very useful for the study of a variety of properties of physical systems in a wide range of applications. For instance, they have been used to approximate results for very short-range potentials, to model several kinds of extra thin structures, to mimic point defects in materials, to study heterostructures, to model impurities in quantum field theory models and, more recently, such potentials played an important role in a reinterpretation of the Casimir effect. Contact interactions may also have unexpected relations with other fields, like group theory.

Mathematically, contact interactions are singular, since they are supported on sets of zero Lebesgue measure. Therefore, to unambiguously define a contact interaction it is necessary to establish the mathematical framework used to address the singularities. One method, inherited from quantum field theory, that is commonly used in the physics literature to deal with the singularities, is to define singular potentials by means of a regularization procedure (often followed by renormalization), that is, as the limit of a sequence of regular functions converging in some sense to the singular potential. The regularization method has been particularly useful in investigating the limit of square potentials and the corresponding point interactions, both in non-relativistic and relativistic quantum mechanics. Another method to properly define a singular interaction uses the theory of self-adjoint extensions (SAE) of symmetric operators. In this case, the wave functions in the domain of the self-adjoint Hamiltonian are completely defined by specifying the boundary conditions they must satisfy at the borders of the singularity. The SAE method provides all the possible self-adjoint extensions allowed for a given symmetric operator and it has been used in a wide variety of models and applications. Yet another approach to define singular interactions is by considering the singular potential (and also the wave function, in some approaches) as a distribution and, by using the apparatus of distribution theory, to define consistently the otherwise ill-defined product of the potential and the wave function in the Schrödinger (or Dirac) wave equation.

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The contributed papers to this Research Topic are original works that use the methods mentioned above (and more) to address not only the theoretical and mathematical aspects of contact interactions, but also their applications to a broad range of fields. Below we present a brief description of these contributions.

Glasser considers a quantum system with known green function and obtains the exact green function for the situation in which two δ-impurities are added to the system. After analyzing various particular cases of the parameters, the author generalizes the result for N such impurities. Kulinskii and Panchenko use the conservation of the current density to obtain the boundary conditions defining a self-adjoint Hamiltonian for the one dimensional Schrödinger operator with spin. These self-adjoint extensions produce point potentials such that the spin is not a constant of motion. The authors also add a physical interpretation to this effect. Dell'Antonio defines contact interactions by boundary conditions at the contact manifold and, by using tools of functional analysis and the gamma convergence, obtains self-adjoint extensions of the free Hamiltonian that correspond to weak and strong contact interactions. The author also illustrates these results in some applications in one, two and three spatial dimensions, which include low and high densities Bose-Einstein condensates and the unitary gas.

Bordag et al. consider a one-dimensional scalar field in the background of a Kronig-Penney potential with a δ-δ' interaction. They obtain the band structure of the model and compute the non-perturbative vacuum energy, using the spectral Zeta-function method. Rabinovich et al. study band spectra of one dimensional systems containing infinite point singularities, each one consisting of a comb of the Dirac delta and its derivative. The self-adjointness of the Hamiltonians is guaranteed by matching the boundary conditions at each singular point. The authors also provide several numerical examples to illustrate the approach. Erman and Turgut consider Hamiltonians perturbed by singular potentials, with support on points and curves, and address the splitting of the bound state energy levels due to quantum tunneling. They show, using Krein's resolvent approach, that the splitting can be obtained perturbatively under certain conditions.

One dimensional Hamiltonians, with electro-magnetic field potentials localized around a point and depending on coupling constants, are studied by Golovaty. By using a limiting procedure that shrinks the supports of these potentials to a single point, the author obtains a potential of the Dirac delta type plus its derivative, if zero energy resonances for one component of the potential exist. The author also shows that such zero energy resonances are solutions of the Schrödinger equation with non-trivial bounded solutions on the whole real line. By using a similar approach, Zolotaryuk et al. start with multilayer regular potentials in one dimension and, after squeezing them by using suitable limiting procedures, obtain point interactions. The authors use a "point" transistor to illustrate the interpretation of the squeezing process as being due to the application of a controllable bias potential. Calçada et al. revisit the one-dimensional Hydrogen atom, which is described by a Coulomb-type long-range potential having a singularity at the origin. The authors use an approach based on the Schwartz theory of distributions and present a systematic study regarding the multiplicity and parity of the bound states and the boundedness of the ground state energy for all the possibilities of self-adjoint parity invariant interactions.

Albeverio et al. consider a two-dimensional system, where the free particle Hamiltonian is perturbed with a harmonic oscillator potential in the x direction, plus a Gaussian potential isotropic in the two dimensions. The resulting Hamiltonian is self-adjoint and bounded from below. By replacing the Gaussian potential in the x direction by a Dirac delta potential the authors obtain a new Hamiltonian, with similar properties to the original one, and also estimate a lower bound for the spectrum. The authors also show that this new Hamiltonian is a limit, in the strong resolvent sense, of a sequence of Hamiltonians of the type studied in the first place. Guilarte et al. present an in-depth investigation of the spectral problem for the Dirac Hamiltonian of one-dimensional electrons and positrons with either electrostatic or position-dependent mass impurities given by a δ-function potential, a necessary analysis for their goal of building a fermionic quantum field theory and computing the Casimir effect for this system. In the framework of a point particle effective field theory, Hayman and Burgess describe a process of particle-conversion mediated by flavor-changing interactions, in which two light scalar particles interact by contact with a heavy point particle. The singularities of the interactions at the worldline of the heavy particle are handled by using regularization and renormalization techniques. The authors also discuss the connection of their model to a model of a single particle dynamics described by a non self-adjoint Hamiltonian.

Salem et al. review two methods based on the theory of self-adjoint extensions and apply them to approach Hamiltonians with a point singularity in (2 + 1) dimensions. They address the problem of a spin-1/2 charged particle with an anomalous magnetic moment in an Aharonov-Bohm potential in a conic space and apply both the methods to obtain a relationship between the parameter of the self-adjoint extension and the physical parameters of the problem. Erman et al. consider one-dimensional systems decorated with either a Dirac delta or its derivative, in both cases multiplied by a time dependent coefficient, and show that this problem may be solved by using the Laplace transform as an intermediate tool so as to obtain the Green function in either case. Some particular cases are analyzed. Finally, Suchanecki investigates the extensions of time operators acting on spaces of generalized functions associated with K-systems as well as the problem of the decomposability of cylindrical elements.

This Research Topic is an up-to-date sample of the main ideas, concepts and methods of the research on contact interactions in quantum mechanics, and received works of some of the most active researchers presently working in this subject. We thank all of them for their valuable contributions.

AUTHOR CONTRIBUTIONS

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

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A Note on the Exact Green Function for a Quantum System Decorated by Two or More Impurities

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The exact Green function is constructed for a quantum system, with known Green function, which is decorated by two delta function impurities. It is shown that when two such impurities coincide they behave as a single singular potential with combined amplitude. The results are extended to N impurities and higher dimensions.

Keywords: quantum green function, delta function potential, contact interaction, Schroedinger equation, quantum graph
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1. INTRODUCTION

The one dimensional harmonic oscillator or square well, for example, for which the energy -dependent Green function $G_0(x, x'; E)$ is known, have been taken for many years as solvable models for semi-conductor quantum wells [1]. Frequently delta function potentials are placed at various points to simulate defects or impurities. In the case of a single impurity potential, $V(x) = \lambda\delta(x - a)$, the Green function for the composite system is known to be [2]

$$G(x, x'; E) = G_0(x, x') + \lambda \frac{G_0(x, a; E)G_0(a, x')}{1 - \lambda G_0(a, a; E)} \tag{1}$$

In this note a corresponding formula is derived for the case $V(x) = \lambda\delta(x - a) + \mu\delta(x - b)$ On the basis of the analogy of the algebraic structure the result is extended to N-impurities and for a standard interpretation of the Dirac delta function, to higher dimension.

2. CALCULATION

We first note that the same argument can be used for the time dependent-, as well as the energy-dependent Green functions, so we shall omit the third argument and write simply $G(x, x')$.

Beginning with the Dyson equation, noting that $G_0(x, y) = G_0(y, x)$

$$G(x, x') = G_0(x, x') + \int G_0(x, y)V(y)G(y, x')dy, \tag{2}$$

where the integration extends over the system domain, one has the set of equations

$$G(x, x') = G_0(x, x') + \lambda G_0(x, a)G(a, x') + \mu G_0(x, b)G(b, x') \tag{3}$$

$$G(a, x') = G_0(a, x') + \lambda G_0(a, a)G(a, x') + \mu G_0(a, b)G(b, x'), \tag{4}$$

$$G(b, x') = G_0(b, x') + \lambda G_0(a, b)G(a, x') + \mu G_0(b, b)G(b, x'). \tag{5}$$

The linear Equations (4) and (5) are easily solved for $G(a,x')$ and $G(b,x')$:

$$G(a,x') = \frac{G_0(a,x') + \mu[G_0(b,x')G_0(a,b) - G_0(a,x')G_0(b,b)]}{D} \tag{6}$$

$$G(b,x') = \frac{G_0(b,x') + \lambda[G_0(a,x')G_0(a,b) - G_0(b,x')G_0(a,a)]}{D} \tag{7}$$

with

$$D = [1-\lambda G_0(a,a)][1-\mu G_0(b,b)] - \lambda\mu[G_0(a,b)]^2. \tag{8}$$

By inserting (6) and (7) into (3) we obtain the desired expression

$$\begin{aligned} G(x,x') &= G_0(x,x') \\ &+\frac{1}{D}\{\lambda G_0(x,a)G_0(a,x') + \mu G_0(x,b)G_0(b,x') \\ &+\lambda\mu[G_0(x,a)\left(G_0(a,b)G_0(a,x') - G_0(b,b)G_0(b,x')\right) \\ &+G_0(x,b)\left(G_0(a,b)G_0(a,x') - G_0(a,a)G_0(a,x')\right)]\}. \end{aligned} \tag{9}$$

3. DISCUSSION

By setting μ to 0 (9) reduces to (1), proving this expression as well. The most salient feature of (9) is the denominator D whose zeros form the exact spectrum of the composite system. For example, when a and b coincide, D reduces to $1-(\lambda+\mu)G(a,a)$ and (9) reduces to (1) with λ replaced by the amplitude $\lambda+\mu$. I.e., the two impurities combine to form one with combined amplitude. This generalizes the result of Fasssari and Rinaldi [3], for two identical defects symmetrically placed with respect to the center of a harmonic oscillator. An expression similar to (9) has been derived recently by Horing (private communication) for the case of a quantum dot in a magnetic field.

Two further points can be made. Nothing in the derivation of (9) restricts it to the line. If we accept the standard definition $\delta(\vec{x}) = \Pi_{j=1}^{d}\delta(x_j)$, then (9), and its consequences, are valid for d-dimensional quantum systems. This has been proven function-theoretically for the three dimensional quantum dot with two symmetrically placed identical impurities by Albeverio et al. [4].

A second observation is that D is simply the Cramer determinant for the pair of simultaneous linear Equations (4) and (5). In the case of impurity potential

$$V(x) = \sum_{j=1}^{N}\lambda_j\delta(x-a_j) \tag{10}$$

there will be N such equations and the determinant is easily evaluated. The general result is

If a quantum system having Green function $G_0(x,y)$ is decorated with N delta function impurities $\lambda_j\delta(x-a_j)$, $j=1,2,\cdots N$, then the new energy levels are the roots of

$$D_N = \prod_{j=1}^{N}A_{jj} - \sum_{j=2}^{N}(-1)^j \sum_{1\le k_1<\cdots k_j\le N} A_{k_1k_2}A_{k_2k_3}\cdots A_{k_jk_1} = 0 \tag{11}$$

where $A_{lm} = \delta_{lm} - \lambda_l G_0(a_l,a_m)$.

Thus,

$$\begin{aligned} D_3 &= \prod_{j=1}^{3}[1-\lambda_j G_0(a_j,a_j)] - \sum_{i<j}\lambda_i\lambda_j G_0(a_i,a_j)G_0(a_j,a_i) \\ &+\lambda_1\lambda_2\lambda_3 G_0(a_1,a_2)G(a_2,a_3)G_0(a_3,a_1), \end{aligned} \tag{12}$$

which reduces to the $N=1$ and $N=2$ cases appropriately and shows that any two coinciding impurities coalesce as indicated above.

Note that if all the λs and a's coincide then

$$D_N = (1-\lambda G_0(a,a))^N - \sum_{j=2}^{N}\binom{N}{j}\lambda^j G_0(a,a)^j = (1-N\lambda G_0(a,a)). \tag{13}$$

Equation (11) might offer a new approach to Kronig-Penney-type systems for periodic or random unit cells.

Finally, it should be pointed out that the work in this note is paralleled in the theory of quantum graphs introduced by Linus Pauling about 1930 to describe electrons in molecules which has developed into a sophisticated and important branch of quantum physics [5]. For relations of this discipline to the present work see the papers by Andrade et al. [6] and Andrade and Severini [7].

AUTHOR CONTRIBUTIONS

The author confirms being the sole contributor of this work and has approved it for publication.

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Point-Like Rashba Interactions as Singular Self-Adjoint Extensions of the Schrödinger Operator in One Dimension

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We consider singular self-adjoint extensions for the Schrödinger operator of spin-1/2 particle in one dimension. The corresponding boundary conditions at a singular point are obtained. There are boundary conditions with the spin-flip mechanism, i.e., for these point-like interactions the spin operator does not commute with the Hamiltonian. One of these extensions is the analog of zero-range δ-potential. The other one is the analog of so called $\delta^{(1)}$-interaction. We show that in physical terms such contact interactions can be identified as the point-like analogs of Rashba Hamiltonian (spin-momentum coupling) due to material heterogeneity of different types. The dependence of the transmission coefficient of some simple devices on the strength of the Rashba coupling parameter is discussed. Additionally, we show how these boundary conditions can be obtained from the Dirac Hamiltonian in the non-relativistic limit.

Keywords: Schrödinger operator, self-adjoint extension, Rashba interaction, spin-flip, Pauli Hamiltonian, Dirac Hamiltonian

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1. INTRODUCTION

Point-like interactions can be described as the singular extensions of the Hamiltonian and are very useful quantum mechanical models because of their analytical tractability [1–5]. They are equivalent to some boundary conditions imposed on a wave function at the singular points and represent the limiting cases of field inhomogeneities. Therefore it is important to understand the relation between parameters of these BC and the specific physical characteristics of inhomogeneities. In modern nanoengineering the spin control is of great interest [6]. Besides the external magnetic field another interaction is the spin-momentum coupling which could be used for such a control [7, 8]. Thus the inclusion of magnetic field and other interactions which influence spin dynamics is a natural route for searching spin-dependent singular interactions. The interactions which influence spin polarization would give new examples of contact interactions with applications in condensed matter physics and QFT [9].

2. CONTACT INTERACTIONS FOR SPIN 1/2 CASE

In non-relativistic limit spin $s = 1/2$ particle is described by the Pauli Hamiltonian [10]:

$$\hat{H} = \frac{\left(\hat{p} - \frac{q}{c}\mathbf{A}\right)^2}{2m} + q\varphi - \frac{q\hbar}{2mc}\hat{\boldsymbol{\sigma}} \cdot \vec{\mathcal{H}}, \tag{1}$$

where $\boldsymbol{\sigma}$ represents the vector of Pauli matrices, $\vec{\mathcal{H}}$ is the external magnetic field and $\mathbf{A}, \varphi$ are vector and scalar potentials correspondingly. This Hamiltonian acts in space of 2-component wave functions:

$$\Psi = \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix}. \tag{2}$$

Here $\psi_\uparrow, \psi_\downarrow$ are the wave functions of corresponding spin "up-" and "down-" states $|\uparrow\rangle, |\downarrow\rangle$. The probability current for Eq. (1) is as following:

$$\mathbf{J}_w = \frac{\hbar}{m}\mathrm{Im}\left(\Psi^\dagger \nabla \Psi\right) - \frac{q}{mc}\mathbf{A}\Psi^\dagger\Psi + \frac{\hbar}{2m}\mathrm{rot}\left(\Psi^\dagger \boldsymbol{\sigma}\ \Psi\right), \tag{3}$$

where the last term describes the magnetization current (see e.g., [11]).

Bearing in mind the application to the 1-dimensional layered systems with spatial heterogeneity we use the conservation of current 3 to derive the boundary conditions (BCs) for the Hamiltonian 1 which model point-like interactions. We use the results of [12] where all possible self-adjoint BCs were related with the following Hamiltonian:

$$L_X = -D_x^2(1 + X_4\,\delta) + i\,D_x\left(2\,X_3\,\delta - i\,X_4\,\delta^{(1)}\right) + X_1\,\delta + (X_2 - i\,X_3)\,\delta^{(1)}. \tag{4}$$

Here symbol D_x stands for the derivative in the sense of distributions on the space of functions continuous except at the point of singularity where they have bounded values along with their first derivatives [12, 13]:

$$\delta(\varphi) = \frac{\varphi(+0) + \varphi(-0)}{2}, \quad \delta^{(1)}(\varphi) = -\frac{\varphi'(+0) + \varphi'(-0)}{2}. \tag{5}$$

The parameters $X_i \in \mathbb{R}$ determine the values of the discontinuities of the wave function and its first derivative. The boundary conditions (b.c.) corresponding to each contribution in Eq. (4) can be represented in matrix form:

$$\begin{pmatrix} \psi(0+0) \\ \psi'(0+0) \end{pmatrix} = M_{X_i} \begin{pmatrix} \psi(0-0) \\ \psi'(0-0) \end{pmatrix} \tag{6}$$

and conserve the current*

$$j = 2\,\mathrm{Im}\left(\psi^*\,\psi'\right) \tag{7}$$

of the Hamiltonian

$$\hat{H} = -\frac{d^2}{d\,x^2} \tag{8}$$

of a spinless particle. Physical classification of all these b.c. on the basis of gauge symmetry breaking was proposed in Kulinskii and Panchenko [14]. They can be divided into two subsets. The first one is formed by the matrices:

$$M_{X_1} = \begin{pmatrix} 1 & 0 \\ X_1 & 1 \end{pmatrix}, \qquad M_{X_4} = \begin{pmatrix} 1 & -X_4 \\ 0 & 1 \end{pmatrix} \tag{9}$$

and can be associated with point-like interactions of electrostatic nature, e.g., standard zero-range potential is nothing but the limiting case of the potential field barrier. Another one is given by the BC matrices:

$$M_{X_2} = \begin{pmatrix} \mu & 0 \\ 0 & 1/\mu \end{pmatrix}, \qquad M_{X_3} = e^{\pi\,i\,\Phi}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{10}$$

and represents the point-like interactions of the "magnetic" type. The parameters of 4 are related with the physical ones:

$$X_2 = 2\,\frac{\mu - 1}{\mu + 1}, \quad e^{\pi\,i\,\Phi} = \frac{2 + i\,X_3}{2 - i\,X_3}, \tag{11}$$

where $\mu = \sqrt{m_+/m_-}$ is the mass-jump parameter and Φ is the magnetic flux (in units of $\Phi_0 = 2\pi\,\hbar\,c/q$). The magnetic nature of M_{X_3} is obvious because of its interpretation as the localized magnetic flux. The last breaks the homogeneity of the phase of the wave function ψ. Also the scattering matrix of this b.c. has no time reversal symmetry [14].

The natural question arises as to the consideration of a particle with internal magnetic moment, e.g., a particle with spin $s = 1/2$. The very straightforward way for derivation of corresponding b.c. is the conservation of current Eq. (3). Therefore we introduce 4-vector (bispinor) of the boundary values at the singular point:

$$\Phi_{0\pm0} = \begin{pmatrix} \psi_\uparrow \\ \psi'_\uparrow \\ \psi_\downarrow \\ \psi'_\downarrow \end{pmatrix}_{0\pm0} \tag{12}$$

and boundary condition 4×4-matrix M:

$$\Phi_{0+0} = M\,\Phi_{0-0}. \tag{13}$$

Due to the structure of current Eq. (3) for the Hamiltonian 1 we have conservation of all its components:

$$\begin{aligned} J_x &= \frac{1}{i}\left(\Psi^\dagger\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^\dagger}{\partial x}\Psi\right), \\ J_y &= -\left(\frac{\partial\Psi^\dagger}{\partial x}\sigma_z\Psi + \Psi^\dagger\sigma_z\frac{\partial\Psi}{\partial x}\right), \\ J_z &= \frac{\partial\Psi^\dagger}{\partial x}\sigma_y\Psi + \Psi^\dagger\sigma_y\frac{\partial\Psi}{\partial x}. \end{aligned} \tag{14}$$

Note that here we use expanded form of "curl" operator in Eq. (3) with explicit derivatives because we expect the discontinuity in their values. In fact, this the very form follows from the Dirac equation in non relativistic limit and the curl-operator appears after collecting the corresponding terms (see [10]). This point is important in view of X_2-interaction which breaks the homogeneity of dilatation symmetry [15] because of the mass jump [14, 16]. In general J_y and J_z are different from zero even if we consider 1-dimensional case, e.g., layered system. The only demand consistent with the hermiticity of the Hamiltonian Eq. (1) is the conservation of current components Eq. (14). In

*here we put $\hbar = 1$, $c = 1$ and $m = 1/2$.

terms of vector Φ the components of the probability current are as following:

$$J_i = \Phi^\dagger \, \Sigma_i \Phi \,, \quad i = x, y, z \tag{15}$$

where 4×4 matrices Σ_i are calculated by comparison of expressions Eqs. (14) and (15):

$$\Sigma_x = \frac{1}{i} \begin{pmatrix} Sp_2 & 0 \\ 0 & Sp_2 \end{pmatrix}, \quad \Sigma_y = \begin{pmatrix} -\sigma_x & 0 \\ 0 & \sigma_x \end{pmatrix}, \tag{16}$$

$$\Sigma_z = \frac{1}{i} \begin{pmatrix} 0 & \sigma_x \\ -\sigma_x & 0 \end{pmatrix} \text{ and } \quad Sp_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{17}$$

The conservation constraint of total current 15 gives the conditions for M-matrix:

$$M^\dagger \, \Sigma_i \, M = \, \Sigma_i \,, \; i = x, y, z \tag{18}$$

Besides trivial solution for M-matrix consisting of two $M_{X_{2,3}}$-blocks (no spin-flip), simple algebra gives the nontrivial 1-parametric solution of Eq. (18):

$$M_r = \begin{pmatrix} 1 & 0 & 0 & r \\ 0 & 1 & 0 & 0 \\ 0 & r & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad r \in \mathbb{R} \tag{19}$$

with

$$M_{r_1} \, M_{r_2} = M_{r_1 + r_2} \,.$$

and b.c. of the form

$$\begin{pmatrix} \psi_\uparrow \\ \psi'_\uparrow \\ \psi_\downarrow \\ \psi'_\downarrow \end{pmatrix}_{0+0} = M_r \, \Phi_{0-0} = \begin{pmatrix} \psi_\uparrow + r \, \psi'_\downarrow \\ \psi'_\uparrow \\ \psi_\downarrow + r \, \psi'_\uparrow \\ \psi'_\downarrow \end{pmatrix}_{0-0} \tag{20}$$

This defines the spin-flip variant of X_4-extension. E.g., corresponding scattering matrix for M_r is as following:

$$\hat{S}_r = \frac{1}{k^2 r^2 + 4} \begin{pmatrix} k^2 r^2 & 4 & -2\,i\,k\,r & 2\,i\,k\,r \\ 4 & k^2 r^2 & 2\,i\,k\,r & -2\,i\,k\,r \\ -2\,i\,k\,r & 2\,i\,k\,r & k^2 r^2 & 4 \\ 2\,i\,k\,r & -2\,i\,k\,r & 4 & k^2 r^2 \end{pmatrix} \tag{21}$$

The scattering characteristics related to the scattering matrix Eq. (21) are in **Figure 1**.

Another solution of Eq. (18) is

$$\tilde{M}_{\tilde{r}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & \tilde{r} & 0 \\ 0 & 0 & 1 & 0 \\ \tilde{r} & 0 & 0 & 1 \end{pmatrix}, \quad \tilde{r} \in \mathbb{R} \tag{22}$$

with the b.c. of the form:

$$\begin{pmatrix} \psi_\uparrow \\ \psi'_\uparrow \\ \psi_\downarrow \\ \psi'_\downarrow \end{pmatrix}_{0+0} = \tilde{M}_{\tilde{r}} \, \Phi_{0-0} = \begin{pmatrix} \psi_\uparrow \\ \psi'_\uparrow + \tilde{r} \, \psi_\downarrow \\ \psi_\downarrow \\ \psi'_\downarrow + \tilde{r} \, \psi_\uparrow \end{pmatrix}_{0-0} \tag{23}$$

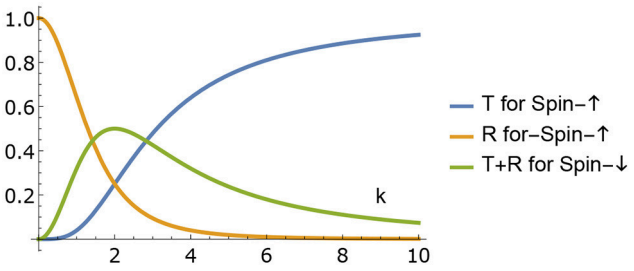

FIGURE 1 | Scattering of $|\uparrow\rangle$ - state on $r - X_4$ defect.

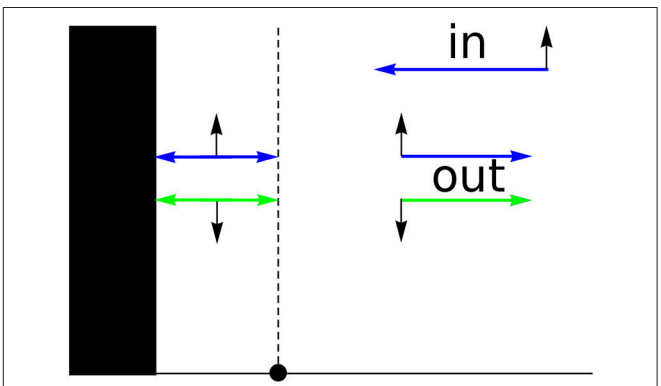

FIGURE 2 | Resonator.

It can be considered as the δ-potential (X_1-extension) augmented with the spin-flip mechanism. From the explicit form of the boundary conditions, e.g.,:

$$\begin{pmatrix} \psi_\uparrow \\ \psi'_\uparrow \\ \psi_\downarrow \\ \psi'_\downarrow \end{pmatrix}_{0+0} = M_r \, M_{X_2} \, \Phi_{0-0} = \begin{pmatrix} \mu^{-1} \, \psi_\uparrow + \mu \, r \, \psi'_\downarrow \\ \mu \, \psi'_\uparrow \\ \mu^{-1} \psi_\downarrow + \mu \, r \, \psi'_\uparrow \\ \mu \, \psi'_\downarrow \end{pmatrix}_{0-0} \tag{24}$$

where M_{X_2} is the block-diagonal matrix of X_2-extensions. Thus the boundary condition for $s = 1/2$ particle with the spin-flip contact interaction can be written in general form:

$$\Phi_{0+0} = \tilde{M}_{\tilde{r}} \, M_r \, M_{X_2} \,. \tag{25}$$

Note that X_3-extension can not be augmented with the spin-flip mechanism since it decouples from $r, \tilde{r}$-couplings. In accordance with the spin-momentum nature of the r-couplings the physical reason of such factorization is that X_3 contact interaction does not include spatial inhomogeneity in electric field potential φ. This is quite consistent with the difference between X_2 and X_3 from the point of view of breaking the gauge symmetry [14, 17].

Using the b.c. obtained above the standard test systems and their transport characteristics can be calculated straightforwardly in order to demonstrate spin-filtering properties. We give just two examples. First is the resonator (see **Figure 2**) for which the scattering amplitudes are in **Figures 3**, **4**. Also we give the

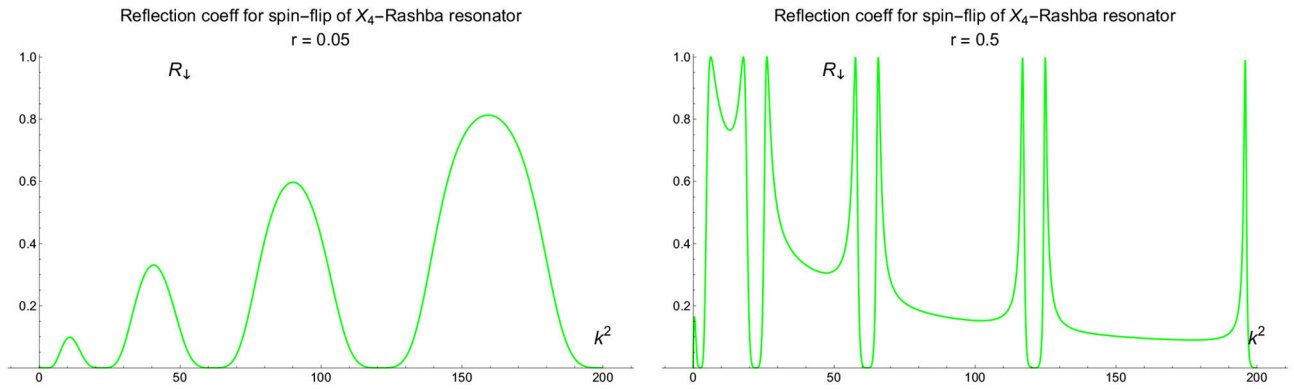

FIGURE 3 | Intensity of reflected spin-↓ state for $r - X_4$ resonator (see **Figure 2**) at different values of r.

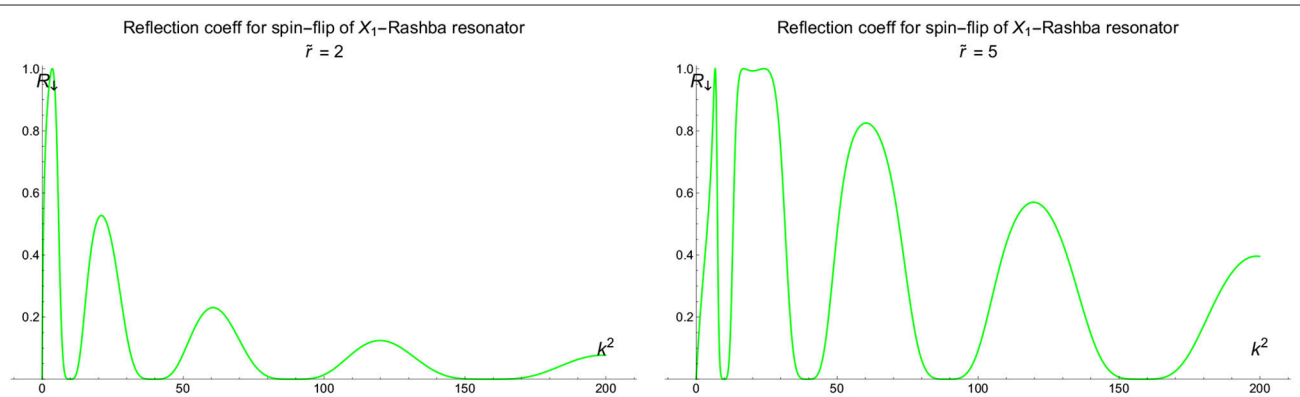

FIGURE 4 | Intensity of reflected spin-↓ state for $\tilde{r} - X_1$ resonator (see **Figure 2**) at different values of $\tilde{r}$.

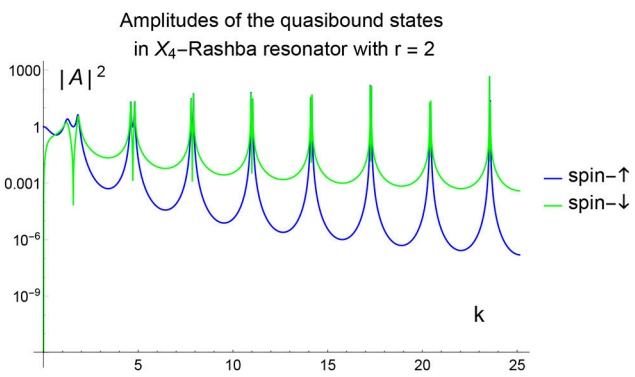

FIGURE 5 | Amplitude of the wave function $|\uparrow\rangle, |\downarrow\rangle$-components in the resonant region.

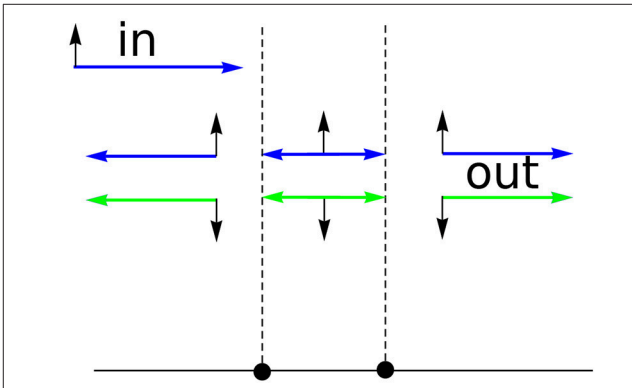

FIGURE 6 | Filter.

results of calculation of the resonant (quasilocalized) states (see **Figure 5**). Second is the filter (see **Figure 6**) with scattering characteristics are in **Figure 7**. The intensity of spin-flip process, generating the spin-↓ state from incident spin-↑ state is shown in **Figure 3**. These results demonstrate that spin-flip mechanism even at small values of r-coupling can reach high probabilities with increasing the energy of incident particle. Of course this directly follows from the boundary conditions (19) and (22) since the effects depend on both r and the momentum. **Figure 4** represents the spin-flip effect for X_1-resonator. Using such device it is possible to create the resonant (quasibound) states in the area between the wall and the defect (see **Figure 5**) for X_4-filter.

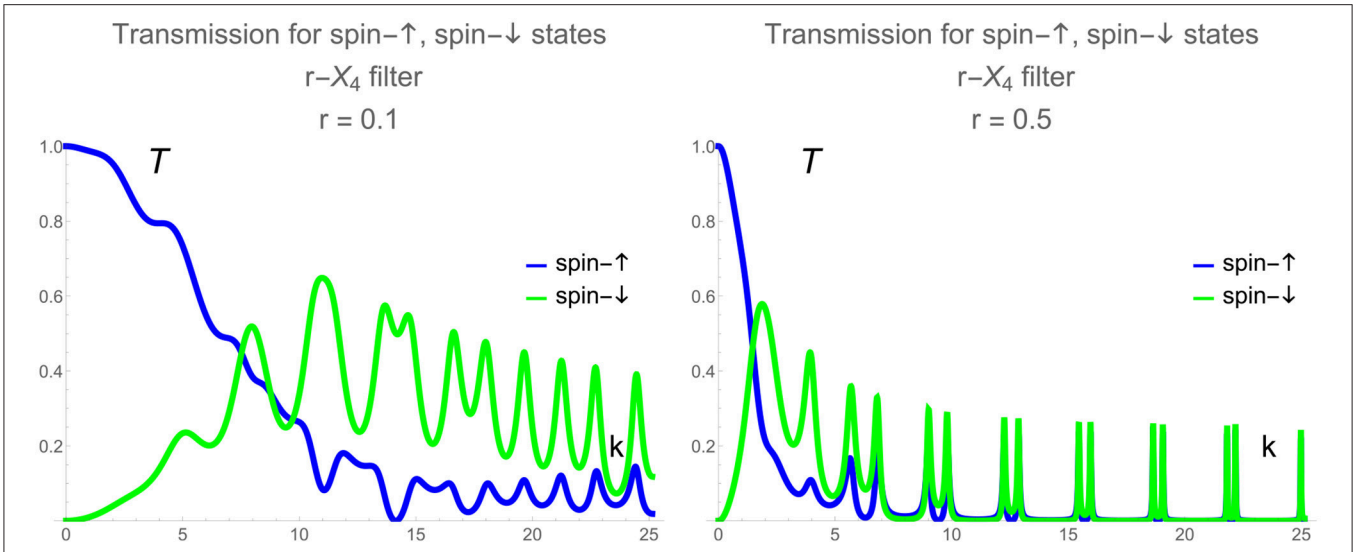

FIGURE 7 | Transmission $r - X_4$ filter intensity for different values of r.

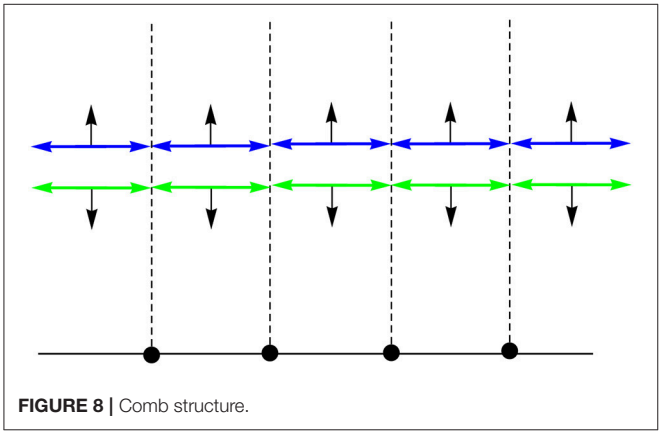

FIGURE 8 | Comb structure.

Comparison of $\tilde{r} - X_1$ and $r - X_4$ cases shows that the last one is more effective as spin-flip mechanism.

The zone structure for periodic comb (see **Figure 8**) can be also calculated in standard way using Bloch representation of the wave function and imposing the corresponding b.c. In comparison with the spinless case considered in Albeverio et al. [3] here the spin degree of freedom doubles the number of zones (see **Figures 9**, **10**). The corresponding dispersion laws are:

$$\cos q = \cos k \pm \frac{r_{X_1}}{2\,k}\,\sin k \tag{26}$$

$$\cos q = \cos k \pm \frac{r_{X_4}\,k}{2}\,\sin k \tag{27}$$

where q is the quasimomentum vector. Note that in case of X_4-comb the lowest states belong to two parabolic zones with different effective masses at $r_{X_4} < 1$:

$$E_{\pm}(k) = \frac{\hbar^2\,k^2}{2\,m_{\pm}}, \quad m_{\pm} = 1 \pm r_{X_4} \tag{28}$$

At $r = 1$ one branch of excitations becomes massless:

$$E(k) = 2\sqrt{3}\,k + \ldots \tag{29}$$

Of course this is the remnant of what happens in standard X_4-structure (see e.g., [3]). More intriguing problem here is the inclusion of the correlation effects due to spin statistics and investigation of phases with magnetic (dis)order in dependence on the intensity of point-like interactions. This way of research may be useful for modeling 1-dimensional magnetic systems [18].

2.1. Spin-Flip Contact Interaction in 3D

As is known 3D case with the spherical symmetry can be effectively reduced to one dimensional problem on semi-axis $r > 0$ of the radial coordinate. Indeed let us define $\phi(r) = r\,\psi(r)$ as the effective 1D wave function and consider natural definition domain of free Hamiltonian:

$$||\hat{H}_0\Psi||^2 = \int_0^{\infty} |(r\,\psi)''|^2 d\,r < \infty \tag{30}$$

then the limiting value $\phi(0)$ as well as its derivative $\phi'(0)$ is defined since Eq. (30) is well defined on the corresponding Sobolev space $W_2^2(\mathbb{R}_+)$ which is dense in $L_2(\mathbb{R}_+)$. The probability current is as following:

$$J = \int_0^{\infty} \mathrm{Im}\left(\Psi^{\dagger}\,\frac{\partial\Psi}{\partial r}\right) r^2\,dr = \int_0^{\infty} \mathrm{Im}\left((r\Psi^{\dagger})\,\frac{\partial(r\Psi)}{\partial r}\right) dr \tag{31}$$

so the results for 1D case can be used. Introducing 2-spinor boundary-value vectors:

$$\Phi = \begin{pmatrix}\phi_{\uparrow}\\ \phi_{\downarrow}\end{pmatrix}, \quad \Phi' = \begin{pmatrix}\phi'_{\uparrow}\\ \phi'_{\downarrow}\end{pmatrix} \tag{32}$$

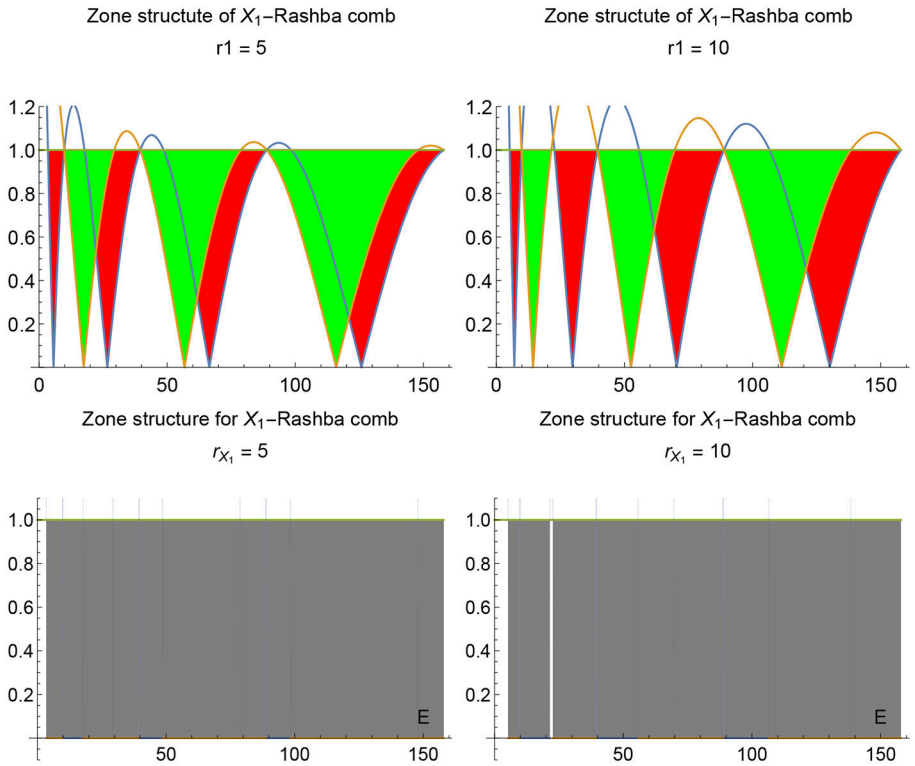

FIGURE 9 | Zone structure of $r - X_1$ - comb. Red and green are for "minus" and "plus" branches in Eq. (26) correspondingly.

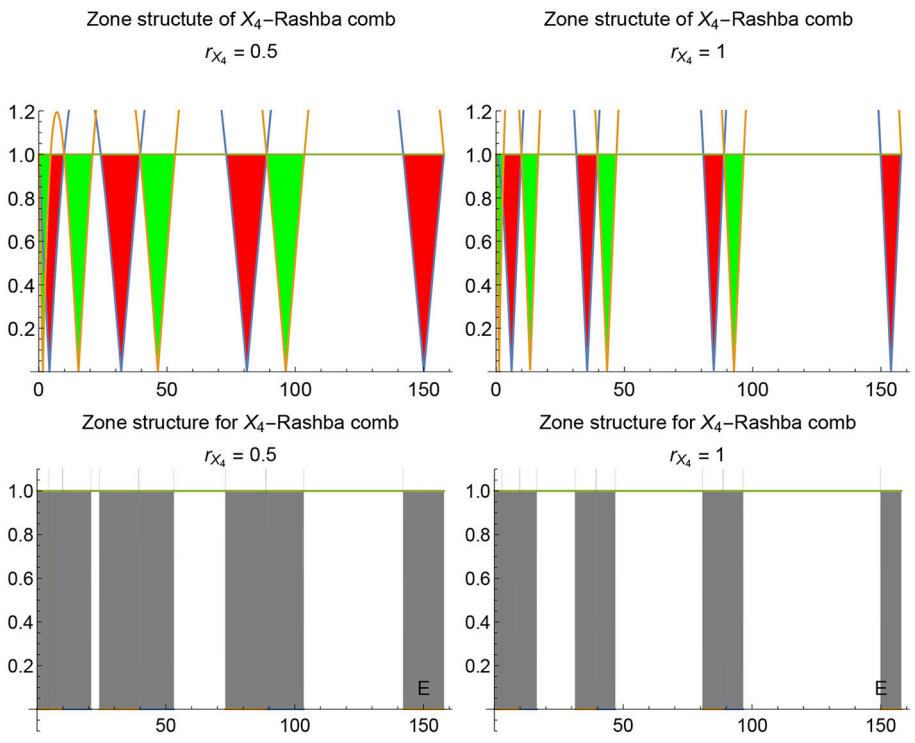

FIGURE 10 | Zone structure of $r - X_4$ - comb. Red and green are for "minus" and "plus" branches in Eq. (27) correspondingly.

where

$$\phi_\alpha = \lim_{r\to 0} r\,\psi_\alpha(r)$$

from Eq. (31) we get:

$$\Phi' = W\,\Phi \tag{33}$$

where W is the hermitean matrix. In standard decomposition on the Pauli matrices:

$$W = \Omega\, I + \mathbf{w}\cdot\boldsymbol{\sigma} \tag{34}$$

the scalar part (first term) corresponds to standard point-like potential b.c. [2, 19]:

$$\Phi' = \Omega\,\Phi \tag{35}$$

and the states $|\uparrow\rangle, |\downarrow\rangle$ evolve independently. There is also spin-dependent repulsive/attractive version of 35:

$$\Phi' = \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \Phi \tag{36}$$

which might be interpreted as the point-like potential with internal spin so that the sign of the potential depends on the spin-spin orientation of the particle and the center. The vector part (traceless second term) of Eq. (34) describes polarizational contact interactions with the spin-flip b.c.:

$$\Phi' = \begin{pmatrix} 0 & z \\ z^* & 0 \end{pmatrix} \Phi\,, \quad z\in\mathbb{C} \tag{37}$$

These b.c.'s in general describe how spin of an incident particle (e.g., an electron) interacts with the electrostatic potential localized at the singular point. In the absence of the external magnetic field the only mechanism for acting on spin in such situation is the relativistic spin-momentum coupling which we discuss in the following section.

3. PHYSICAL ORIGIN OF THE SPIN-FLIP BOUNDARY CONDITIONS

The spin-flip point interactions introduced above make the spin operator no longer the integral of motion. There are two obvious physical origins for it (a) an external magnetic field with x, y-components and (b) spin-momentum coupling (Rashba coupling). The explicit k-dependence of the amplitudes of the spin-flip processes indicates that these interactions are due to spin-momentum coupling. Thus the physical interpretation of interactions represented by the b.c. matrices $M_r, \tilde{M}_{\tilde{r}}$ can be given in terms of the Rashba Hamiltonian [7, 8] (see also [20] and reference therein). Indeed, the Pauli Hamiltonian Eq. (1) as well as the current density Eq. (3) can be derived as the non relativistic limit for the Dirac Hamiltonian

$$\hat{H}_D = \boldsymbol{\alpha}\cdot\left(\hat{\mathbf{p}} - \mathbf{A}\right) + \beta\, m + \varphi \tag{38}$$

where $\boldsymbol{\alpha} = \alpha_i$, $i = 1, 2, 3$ and β are the Dirac matrices

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \tag{39}$$

with I being 2×2 unit matrix. They act in the space of bispinors Ψ:

$$\Psi_D = \begin{pmatrix} \xi \\ \eta \end{pmatrix} \tag{40}$$

where spinors ξ and η represent particle and hole with respect to the Dirac vacuum states respectively [10]. The probability density is:

$$\mathbf{J}_D = \Psi_D^\dagger\,\boldsymbol{\alpha}\,\Psi_D \tag{41}$$

and in non relativistic limit transforms into

$$\mathbf{J} = \xi^*\,\boldsymbol{\sigma}\,\eta + \eta^*\,\boldsymbol{\sigma}\,\xi \tag{42}$$

with

$$\eta = \frac{1}{2\,m}\hat{\mathbf{v}}\,\xi \tag{43}$$

Here $\hat{\mathbf{v}}$ is the velocity operator. In the absence of external electromagnetic field this is equivalent to the following reduction of the bispinor in 1-dimensional case

$$\Psi_D \to \begin{pmatrix} \xi \\ \xi' \end{pmatrix} \tag{44}$$

so that the boundary element 4-vector 12 appears. Also we refer to the paper [21] where mass jump matching conditions were derived for the Dirac Hamiltonian in a graphen-like material where the velocity v_F at the Fermi level serves as the speed of light.

The expansion of next order generates the spin dependent operator in the Hamiltonian:

$$\hat{H}_{SP} = \lambda\,\boldsymbol{\sigma}\cdot\left(\nabla\varphi\times\hat{\mathbf{p}}\right) \tag{45}$$

It couples the spin with the momentum due to inhomogeneous background of the electric potential φ. In the limiting case of point-like interaction on the axis when $\nabla\varphi \to 0$ on both sides of the singular point this term drops out and should be interchanged with the boundary condition for the boundary vector 12 of the Pauli Hamiltonian 1. The conservation of the corresponding probability density current Eq. (3) provides self-adjointess of the boundary conditions for Eq. (1) in the presence of point-like singularity.

As a result, all extensions X_i, $i = 1, 2, 4$ which are singular limiting cases of the spatial distribution of the external electric field potential φ can be augmented with the spin-flip mechanism. Thus Eq. (25) defines the one-dimensional analog of the Hamiltonian with the point-like Rashba spin-momentum interaction [7].

4. CONCLUSION

The main result of the paper is that those extensions of the Schrödinger operator which are physically constructed on the basis of the inhomogeneous distribution of the electric field

potential $\varphi(x)$ can be augmented with the spin-flip mechanism. Note that in Eq. (24) both r-coupling and μ-parameter determine the spin-flip mechanism. This is in coherence with the results of Kulinskii and Panchenko [17] where X_2 and X_4 extensions were treated on the common basis of the spatial dependent effective mass. In its turn it is caused by the electrostatic field of the crystalline background. So it is not a surprise that these extensions can be combined through spin-momentum coupling in the Rashba Hamiltonian thus forming the "internal" magnetic field. In contrast to this pure "magnetic" X_3-extension which is due to the external magnetic field does not couple with other Rashba point-like interactions.

Thus we can state that all point-like interactions δ, δ'-local and δ'-nonlocal (in terms of [22]) which are due to inhomogeneous electrostatic background can be augmented with the Rashba (spin-momentum) coupling. It is interesting to check this result independently using the Kurasov's distribution theory technique [12] and modified correspondingly for spin 1/2 case. Also we expect that such b.c.'s can be related to the zero-range potential models with the internal structure of the singular point studied in Pavlov [23]. This will be the subject of future work.

AUTHOR CONTRIBUTIONS

VK and DP conceived of the presented idea. VK proposed physical interpretation for the spin-flip matching conditions. VK encouraged DP to investigate the possibility to derive them based on the Dirac Hamiltonian and supervised the findings of this work. All authors discussed the results and contributed to the final manuscript.

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Contact Interactions and Gamma Convergence

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We introduce contact interactions defined by boundary conditions at the *contact manifold* $\Gamma \equiv \cup_{i,j}\{x_i = x_j\}$. There are two types of contact interactions, weak and strong. Both provide self-adjoint extensions of $\hat{H}_0$ the free hamiltonian restricted away from Γ. We analyze both of them by "lifting" the system to a space of more singular functions: the map is fractioning and mixing. In the new space we use tools of Functional Analysis. After returning to physical space we use Gamma convergence, a well-known variational tool. We prove that contact interactions are strong resolvent limits of potentials with finite range. Weak contact of one boson with two other bosons leads to the low-density Bose-Einstrin condensate. Simultaneous weak contact of three bosons produces the high-density condensate which has an Efimov sequence of bound states. In Low Energy Physics strong contact of one particle with another two produces an Efimov sequence of bound states (we will comment briefly on the relation with the effect with the same name in Quantum Mechanics). For N bosons strong contact gives a lower bound $-CN$ for the energy. A system of fermions in strong contact (unitary gas) has a positive hamiltonian. We give several examples in dimension 3,2,1. In the Appendix we describe the ground state of the Polaron.

Keywords: contact, gamma convergence, interaction, Efimov, Bose Einstein

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1. INTRODUCTION

In Classical Mechanics constraints we describe forces restricting the motion of two systems when they are in contact.

In Quantum Mechanics it is convenient to use the Heisenberg representation and describe the system by means of self-adjoint operators on some function space. Each self-adjoint operator has a domain of definition.

We consider first in some detail the dynamics in R^3 and later consider the case of dimension two and dimension one.

Contact (zero range) interactions in R^3 are defined by imposing that the wave function in the domain of the hamiltonian satisfies at the *coincidence manifold* Γ

$$\Gamma \equiv \cup_{i,j}\Gamma_{i,j} \qquad \Gamma_{i,j} \equiv \{x_i - x_j\} = 0, \quad i \neq j \, x_i \in R^3. \tag{1}$$

the boundary conditions

$$\phi(X) = \frac{C_{i,j}}{|x_i - x_j|} + D_{i,j} \quad i \neq j \tag{2}$$

These conditions were used already in 1935 by Bethe and Peirels [1] in the description of the interaction between a proton and neutron.

They were later used by Ter-Martirosian and Skorniakov [2] in their analysis of the three-body scattering within the Faddeev formalism. We shall call them Ter-Martrosian [2] boundary conditions. In the weak contact case *for each contact there is a zero-energy resonance* i.e., a function that *at infinity* is proportional to $\frac{1}{|x_i - x_j|}$.

For contact interactions it is easy to determine the spectra; the interest in the subject was renewed in Theoretical Physics by recent advances in the theoretical formulation of low energy physics and also by the flourishing of research on ultra-cold atoms interacting through potentials of very short range.

The T-M boundary conditions can be described by potentials $V_{i,j}(|x_i - x_j|)$ and $U_{i,j}(|x_i - x_j|)$ hat are *distributions supported by the boundary*

$$V_{i,j} = -C_{i,j}\delta(x_i - x_j) \quad \frac{d}{d\rho_{i,j}} U_{i,j}(\rho_{i,j}) = -D_{i,j}\delta(x_i - x_j)$$
$$C_{i,j} > 0 \;\; D_{i,j} > 0 \qquad \rho_{i,j} = |x_i - x_j| \qquad (3)$$

This can be verified by taking the scalar product with a function in the domain of $\hat{H}_0$ (the free hamiltonian restricted to functions that vanish in a neighborhood of Γ) and integrating by parts.

This condition implies a *very singular modification of the free dynamics* at coincidence hyper-planes.

At the boundary, the solutions are not in the domain of the free hamiltonian; *solution of the Schrödinger equation* is only meant in a weak sense, after averaging with a smooth function and integrating by parts.

The equation holds *in the sense of quadratic forms*. Quadratic form techniques play an important role.

2. STRONG AND WEAK CONTACT

We call *strong contacts* the self-adjoint extension characterized by $D_{i,j} = 0$ and *weak contacts* the one characterized by $C_{i,j} = 0$.

From a mathematical point of view, the resulting operators are *self-adjoint extensions* of the symmetric operator $\hat{H}_0$, the free hamiltonian for three particles of mass m defined on functions that have support away form Γ.

Notice in the case of strong contact both the free hamiltonian and the potential define quadratic forms (of opposite sign) on absolutely continuous functions.

The (negative) potential is defined on the larger class of continuous functions and there takes a finite value.

On continuous functions that are not absolutely continuous the quadratic form of the free hamiltonian "is infinite."

Therefore, in a two-particle system strong contact cannot be defined.

Weak contact can be defined but its domain contains a zero-energy resonance.

We shall prove that in three particle system *separate* strong contact of one particle with two other particles can be defined.

If the potential is sufficiently strong the system has an Efimov spectrum.

We consider mainly the case in which all particles have the same mass. In the case of strong contact of one of the particles with the other two the spectrum of Efimov type.

A small difference in the masses does not change the structure of the spectrum.

The (energy) scale is given by the mass and by the ratio between the strong and weak contact coefficients, if they are both present.

In the case of weak contact, the distributional potential at the boundary has the same scaling property under dilation as the kinetic energy. Therefore, the hamiltonian of weak contact is scale covariant under the dilation group.

This by itself is an indication of the presence of a resonance. Point interactions [3] can be seen as a weak contact interaction between two particles one of which is infinitely massive (with wave function concentrated in a point).

We emphasize that both strong and weak contact hamiltonian are needed to classify completely the zero range interactions.

We will prove that they produce *complementary and independent effects*.

Both effects are independent from those due to the possible presence of regular potentials (that may cause further resonances).

For the proof of independence, we shall use a general form for the resolvent of the interacting system, due to Krein (we use the Konno and Kuroda [4] improved version).

It should be noted that there is another "natural" extension of $\hat{H}_0$ which is obtained by imposing Dirichlet boundary conditions on some or all contact, manifold.

Imposing Dirichlet boundary conditions is an alternative procedure and *does not correspond* to the limit of attractive potentials V^ϵ.

Remark: To make a connection with the interaction trough two-body potentials, we will prove that the three-body strong contact hamiltonian is limited, in a strong resolvent sense, to Hamiltonians with two body potentials that scale as $V^\epsilon(|x|) = \frac{1}{\epsilon^3} V(\frac{|x|}{\epsilon})$.

Two body weak contact is the limit, in strong resolvent sense, of hamiltonian with potentials that scale as $U^\epsilon(|x|) = \frac{1}{\epsilon^2} U(\frac{|x|}{\epsilon})$ and have a zero energy resonance.

We will show that *in general* (and not only for point interactions [3]) weak contact requires the approximating hamiltonians to have a zero-energy resonance (infinite scattering length).

Since in the case of contact interactions the spectra and spectral properties can be given explicitly, contact interactions are a valuable tool for very short-range potentials.

We shall analyze in detail the case of the separate strong contact of a particle with other two (all particles have the same mass) and the case of the (weak) contact between two pairs of particles which are themselves in strong contact.

With the same formalism we analyze the case of three particles in which every particle has a weak contact interaction with the other two.

Notice that *simultaneous strong contact* of three particles leads to divergences [5].

3. MATHEMATICAL FORMULATION

From a mathematical point of view the problem of zero range interaction between three particles was first analyzed by Pavlov [6] who investigated the self-adjoint extensions defined by the condition that the wave function takes a finite value at the boundary $\Gamma_{i,j}$ (weak contact).

The problem was later studied by Minlos [7, 8] concentrating on (the physically relevant) case of two identical particles one interacting through "zero range potentials" with a particle of the same mass.

The same analysis applies to a system of three identical particles in which each has a strong contact with the other two. For the sake of simplicity all particles have mass one.

To analyze the system, we introduced a compact invertible map (the Krein map $\mathcal{K}$) to a space *of more singular functions*. The map depends on a positive parameter λ; this parameter will play a role in the semiclassical limit.

We call the map "Krein map" $\mathcal{K}$ because our steps are in the path of the theory of self-adjoint extensions of positive operators by Birman [9] and Krein [10], *but on the side of quadratic forms* as suggested in Klaus and Simon [11] (the advantage of this formalism is also remarked in Cassano and Pizzichillo [12]).

The idea of using this map came from reading [7, 8] and therefore we will call Minlos space $\mathcal{M}$ the image space.

The Krein operator is $(H_0 + \lambda)^{-\frac{1}{2}}$.

The Krein map *acts differently* on the kinetic term and on the potential tem.

It acts on the kinetic energy (seen as operator) as follows $(H_0 + \lambda) \to (H_0 + \lambda)^{\frac{1}{2}}$.

It acts on the delta potential (seen as quadratic form) as follows $\delta \to (H_0 + \lambda)^{-\frac{1}{2}} \delta (H_0 + \lambda)^{-\frac{1}{2}}$.

Since for strong and weak contact the distributional potential "commutes" with the free hamiltonian (as seen by taking the Fourier transfor) in $\mathcal{M}$ the quadratic form is also the quadratic form of $\delta(H_0 + \lambda^{-1}$ and this shows a formal relation with Birman [9] and Krein [10].

For very short distances the Krein map enhances the potential term with respect to the kinetic energy.

As a consequence, the quadratic form kinetic energy + potential may become unbounded below (the potential is attractive).

Notice that the Krein is invertible; after inversion, the system was not changed.

The Krein map is only a tool to extract information, a magnifying glass

We distinguish between two cases.

a) Weak contact
   If in $\mathcal{M}$ the result is a unique strongly closed quadratic form, by rotation invariance it can be decomposed into *strictly convex* quadratic form.
   Their image under inversion of the Krein map are weakly closed strictly convex quadratic forms.
   Since the forms are bounded below (the inversion changes the topology of the space) they can be closed strongly [13] and define self-adjoint operators in "physical" space.
   Depending on the strength of the potential there may be a finite number of bound states.
b) Strong contact
   In position space in for $l = 0$ by construction the potential term is the sum of a first order pole (with negative coefficient $-C_0$) and a smooth positive quadratic form Ξ_0 which is zero on the diagonal.
   The form Ξ_0 corresponds to a bounded positive operator; its contribution can be analyzed using perturbation theory.
   Since the Krein map is only an instrument to evidence *general features* of the interaction term *at small distance*, such bounded operators play no role in the following. We shall therefore neglect it.

If C_0 is sufficiently large one has a Weyl limit circle degeneracy [14] and a one-parameter family of self-adjoint extensions all unbounded below and each with an infinite negative point spectrum that diverges linearly. Inversion of the Krein map gives a family of quadratic forms *that are only weakly closed* and bounded below.

If there is one which admits a strong closure, this form defines a self-adjoint operator in physical space with an Efimov spectrum.

This form is obtained using Gamma convergence, a procedure often used in the analysis of finely fragmented materials (we will give later the definitions).

It is a minimization procedure for families of strictly convex forms (not necessary quadratic).

Gamma-convergence selects from a sequence of *strictly convex* forms, a unique one that has a strong closure. This selected form is called Gamma limit. The name *Gamma limit* is used because Gamma convergence is *a minimization process*.

Recall that the Gamma limit of a sequence of *strictly convex* weakly closed forms F_n in a topological space Y is the *unique* weakly closed quadratic form F such that for any subsequence the following holds

$$\forall y \in Y, \quad y_n \to y, \quad F(y) \leq liminf F(y_n) \quad limsup F(y_n) \geq F(y) \tag{4}$$

The limited form is strictly convex and therefore strongly closable.

The condition for the existence of the Gamma-limit is that the sequence be contained in a compact set of Y. In the present case Y has the Frechet topology given by Sobolev semi-norms.

Compactness of bounded sets is assured *by the absence of zero energy resonances*,

Therefore, there is a minimizing (Palais-Smale) sequence.

From the point of view of Functional Analysis, it is important that *Gamma convergence implies resolvent convergence* [15].

Notice that *this is precisely what is done in the study of composite materials: one first acquires information on the "small scale structure" and then draws conclusions at a macroscopic scale*.

We have noticed that the Krein map is *fractioning and mixing*.

This explains why inverting the Krein map requires tools from the theory of homogenization (Gamma convergence

[15]) a procedure often used in the analysis of finely fragmented materials.

If the interaction is strong enough there is an Efimov sequence of bound states.

It is easy to verify that these states (called "trimers" in the Physics literature) have increasingly larger essential support.

Therefore, only the first few members of the series can be detected experimentally.

For an outlook on experimental and theoretical results on the three and four body problem one can consult [16, 17].

4. STRONG AND WEAK CONTACT INTERACTIONS AS LIMITS

a) Strong contact

We prove that strong-contact hamiltonians are limited *in a strong resolvent sense* of finite range hamiltonians.

This makes contact hamiltonians a valuable tool in the study of interactions of a very small range.

We require that the potential $V(|x|)$ be of class C^1. It defines therefore a quadratic form in $\mathcal{H}^1$.

By duality, it is a bounded map from $\mathcal{H}^2$ to C^1 (this explains why we find hamiltonians that are bounded below).

We consider separately the restriction to irreducible representation of the rotation group (the approximating potentials are invariant under rotation).

The quadratic form associated to the potentials V^ϵ is a decreasing function of ϵ (the potential is negative).

Since there is no zero-energy resonance the sequence of the approximating hamiltonians belongs to a compact subset for topology given by the Sobolev semi-norms.

The potential V is negative therefore for any choice of $V \in C^1 \cap L^1$ the ϵ-dependent quadratic forms are *stricly* decreasing as function of ϵ.

A lower bound is the quadratic form of the contact interaction.

A decreasing sequence in a compact set with a lower bound always admits a converging subsequence.

If the sequence is strictly decreasing the limit point is unique.

If the potential is of class C^1 the limit of this converging minimizing subsequence belongs to the limit set of the contact interactions.

Since this set contains only one element for any choice of the L^1 norm of the approximating potentials, the limit is unique and coincides with the contact interaction with the same strength.

Gamma convergence implies strong resolvent convergence [15]. Therefore the sequence of self-adjoint operators with potentials $H_0 + V^\epsilon$, $V^\epsilon \in C^1$ have in strong resolvent sense a limit which is the resolvent of the strong contact hamiltonian (which depends on the L^1 norm of the approximation potentials but *not on the shape*).

In turn strong resolvent convergence implies convergence of spectra and of the Wave Operator in Scattering Theory.

We have proved

Theorem 1: The hamiltonian of a system describing the strong contact interactions of a particle with two identical bosons is limit, in the strong resolvent sense, of hamiltonians with two body *negative* potentials of class C^1 that have support that shrinks to a point with law $V^\epsilon(|x|) = \frac{1}{\epsilon^3} V(\frac{|x|}{\epsilon})$. The limit hamiltonian is bounded below.

There are constant C_1, C_2 such that if $|V|_1 < C_1$ the negative spectrum is empty, if $C_1 \leq |V|_1 < C_2$ the strong contact hamiltonian has a finite negative spectrum while if $|V_1| \geq, C_2$ the negative spectrum is of Efimov type (the sequence of eigenvalues converges geometrically to zero).

In this latter case the eigenfunctions are centered on the barycenter of the system and have increasing support. ◇

Remark: The same is true with the same proof in a three-particle system in which each pair has a separate strong contact interaction.

b) Weak contact

In the case of weak contact, the proof does not apply because the domain of the limit operators contains a zero-energy resonance and compactness in the topology of the Sobolev semi-norms fails.

This is the reason why the approximating potentials V must have a zero-energy resonance.

Since the potentials V^ϵ are obtained by scaling the resonance is independent from ϵ and can be chosen to be the same as the resonance of the weak contact hamiltonian.

Therefore, the domain of difference between the approximating potentials and the weak contact is inL^2 and one has compactness in the Sobolev semi-norms.

5. THE BIRMAN-KREIN-SCHWINGER FORMULA

The role on Gamma convergence in Quantum Mechanics is clearly seen considering the Birman-Krein -Schwinger formula for the difference of the resolvents of two self-adjoint operators H and H_0 both bounded below.

$$(H + \lambda)^{-1} - (H_0 + \lambda)^{-1}) = (H_0 + \lambda)^{-1} W_\lambda (H_0 + \lambda)^{-1} \quad (5)$$

where λ is greater than the lower bound of the spectra.

W_λ is the *Krein kernel*, the quadratic form of a symmetric operator.

Usually H_0 is the free hamiltonian, but one can make other choices (for example H_0 may be the magnetic free hamiltonian, a positive operator).

The B-K-S formula, which is the basis for a perturbative analysis, clearly shows the role of Gamma convergence for strong contact in a non-perturbative setting.

This formula can be written as

$$(H + \lambda)^{-1} - (H_0 + \lambda)^{-1}) = \{K_\lambda\}\{K_\lambda\} W_\lambda) \quad (6)$$

where $\{K_\lambda\}$ is the Krein map.

This formula is ill-defined as it stands because the image of the Krein map is a *weakly closed form* and the Krein map is defined only for strongly closed forms (self-adjoint operators).

If the image is closable in the strong topology one can take its closure before the second Krein map.

If not, one must select one of the weakly closed forms that has a strong closure.

Gamma convergence is the instrument to make this selection.

In the more general setting the formula should be replaced by

$$(H+\lambda)^{-1} - (H_0+\lambda)^{-1}) = \{K_\lambda\}\Gamma(\{K_\lambda\}W_\lambda) \tag{7}$$

where the symbol Γ indicates that it is necessary to use Gamma convergence.

6. BOUNDARY CHARGES

An important aspect of contact interactions is that they are extension of H_0 that are *entirely due to "charges at the boundary."*

In the present case the boundary is *internal* i.e., they are the *contact manifolds*.

Compare with electrostatics: in that case the boundary has co-dimension one and the Krein map can be identified with the Weyl map from potentials to charges.

It is therefore natural to refer to Minlos space as the space of charges [18].

The distribution of "charges at the boundary" determine uniquely the self-adjoint extension; each function in the domain can be written as the sum of a part determined by the charges and a regular part in the domain of H_0. We sketch here the proof.

Let H be the self-adjoint extension that represent the contact interaction.

Choose λ in such a way that $H+\lambda I$ is invertible.

By construction, the quadratic form of $H+\lambda$ is the sum of the quadratic form of $H_0+\lambda$ and a quadratic form in Krein space.

The elements in the form domain of the contact hamiltonian H are of the form $\psi = \phi + \zeta$ where $\phi \in D(H_0)$ and ζ is in Krein space [11].

The action of H on elements in its domain is

$$(H+\lambda)\psi = (H_0+\lambda)\phi \qquad \psi = \phi + \{K_\lambda\}\psi \tag{8}$$

The formal proof (modulo control of the domains) is as follows

$$\begin{aligned}&((H+\lambda)\psi, \frac{1}{H_0+\lambda}(H+\lambda)\psi)\\ &\quad= ((H_0+\lambda)\phi, \frac{1}{H+\lambda}(H_0+\lambda)\phi)\\ &\quad= (\phi,(H_0+\lambda)\phi) + (\{K_\lambda\}\phi, W_\lambda\{K_\lambda\}\phi)\end{aligned} \tag{9}$$

This is same procedure as for finite range potentials; Gamma convergence substantiates this formal argument.

Therefore, only "the space of charges" enters in the description of the domain.

Notice the analogy with electrostatics; the singular part is determined by the charges. The Weyl map takes the role of the Krein map. ♡

7. SOME REMARKS

I

It is worth stressing the connection with the *theory of boundary triples* [19].

This a generalization of the Weyl map in electrostatics from potential in a bounded set Ω in R^3 with regular boundaries to charges at the boundary $\partial\Omega$.

In this context the Krein map may be regarded as a Weyl map between "potentials" and "charges" (the charges belong to a space of more singular functions).

But in the present setting the "boundary charges" are placed on a boundary of co-dimension three (the contact manifold) and not on an external boundary of co-dimension one as in electrostatics (and in most of the papers on boundary triples).

For contact interactions the boundary *is internal* [20].

II

As is often the case for variational arguments for quadratic forms, the eigenfunctions of the minima *are not in the domain of the free hamiltonian*.

The minimum is obtained "by compensation" of the divergences of the kinetic and the potential contributions.

Since the eigenstates *are not in the domain of* H_0 *perturbation theory does not apply*.

The solutions of the Schrödinger equation with contact interaction belong to the space Ξ of functions that are at any time twice differentiable (more precisely in $\mathcal{H}^2$) away from the contact manifold but have a $\frac{1}{|x_i - x_k|}$ singularity at the contact manifold.

Since the Schrödinger flow is dispersive the entire set of solutions has this property.

Bound states are critical points of the energy functional (as in the classical case). Scattering and Wave operators are defined in the space Ξ.

III

It worth recalling that Gamma convergence gives simple results but since it is not a perturbative method it is difficult to evaluate the error made in using contact interactions. The error is of second order in ϵ (it is a minimization process) but the coefficient is not determined.

In the application to nuclear physics a comparison with experimental data [16, 17, 21] gives a reasonable agreement.

IV

One can take the limit in which the two masses of the particles that are not in contact is taken to be infinite; the resulting system is a particle in strong contact with two fixed points (a two-point interaction).

Also, this system has no zero-energy resonance.

On the contrary one cannot assign infinite mass to the particles which interact separately with the two other particles (two identical particles in strong contact with a fixed point); the procedure we follow gives in this limit a divergent result.

8. ON THE ROLE OF GAMMA CONVERGENCE

It is surprising that a formalism invented by de Giorgi more than 50 years ago to handle singular variational problems, and of common use in applied mathematics (and in industry) to treat finely fractured materials, plays an important role in such diverse fields as in the construction of self-adjoint extensions of positive symmetric operators, in the determination of the Efimov structure of three and four bodies systems in high energy physics, in explaining the role of zero energy (Fesbach) resonances (and the secret of the missing $\frac{1}{N}$) in the dilute case of Bose Einstein condensates and in finding the structure of the ground state in at high density.

9. SEMICLASSICAL LIMIT

The energy form for a three-body problem in which all particles have equal mass and each particle has a strong contact interaction with the other two can be evaluated on coherent states centered on the points x_i, $i = 1, 2, 3$ and with "classical momentum" p_1, p_2, p_3.

The result is the "classical" energy functional of the newtonian three body problem.

The hamiltonian of the classical three-body problem admits infinitely many periodic solutions which correspond to critical points of the classical energy functional. Their energy decreases geometrically.

The three-body problem and its periodic solutions are well studied in Classical Mechanics.

In quantum mechanics for identical bosons in strong pairwise contact interactions there is an Efimov sequence of bound states i.e., infinite sequence of bound states with negative eigenvalues that decrease geometrically to zero (as in the classical case).

These are critical points of the quantum energy functional.

This suggests that the classical newtonian three body problem be the semiclassical limit of the quantum mechanical problem of strong contact interaction of one particle with the other two in a system of three identical particles.

Notice that variational problems are studied *using quadratic forms* (and not operators).

In the next section we shall show that the Krein map is related to the semiclassical limit.

10. RELATION OF THE KREIN MAP WITH SEMICLASSICAL LIMIT

We have indicated that in Milnos space the kinetic part of the hamiltonian is represented by $\sqrt{H_0 + \lambda}$ for some (arbitrary) positive λ.

In the three-body problem with strong contact in $\mathcal{M}$ the contact potential is represented by the quadratic form of an attractive Coulomb potential.

For the Krein map we can choose $\lambda > 0$ with the only requirement that the operator $H + \lambda$ is positive.

For λ large on can develop on a dense domain the square root as

$$\sqrt{H_0 + \lambda} = \sqrt{\lambda} + \frac{1}{2}\frac{H_0}{\sqrt{\lambda}} + O(\lambda^{-\frac{3}{2}}) \tag{10}$$

Setting $\frac{1}{\sqrt{\lambda}} = \hbar$, apart from an irrelevant constant, this is to first order in $\hbar$ the free hamiltonian of the quantum system.

When evaluated on coherent states this is the classical free hamiltionian.

When λ is large, in $\mathcal{M}$ strong contact potentials are represented by the Coulomb potential $-\frac{C}{|x_i - x_i|}$ $C > 0$.

Therefore, for λ very large the map $\mathcal{K}_\lambda$ can be related to a semi-classical limit and in $\mathcal{M}$ the free hamiltonian tends (a part for a large constant) to the Classical hamiltonian.

In the semiclassical limit the free hamiltonian is scaled by a factor to $\hbar^{-2}$ and the Coulomb potential is scaled by a factor $\hbar^{-1}$.

If we identify the radius of the potential (the parameter ϵ) with $\hbar$ (both have the dimension of a length) the limit $\hbar = \epsilon \to 0$ gives contact interaction at a quantum scale, Coulomb interaction at a semiclassical scale.

Therefore, the Newtonian three body problem can be considered semiclassical limit of the quantum three body problem with pairwise strong contact interaction.

Addition of a magnetic potential is represented as usual with the substitution $i\nabla \to i\nabla + A$.

11. WEAK CONTACT

Now we consider the case of weak contact.

Since the weak contact potential has the same scaling properties under dilations as the kinetic energy in order to have an hamiltonian which is bounded below there can be at most as many weak contacts as particles.

In R^3 with Riemann stricture weak contact of two particles as self-adjoint extension can occur *only if there is a zero-energy resonance* (infinite scattering length for the approximation potential).

If one of the particles has infinite mass (so that it may be considered as a fixed point) weak contact is called *point interaction*.

In Adami et al. [22], it is proved that this extension cannot exist in a three-dimensional manifold with a sub-Riemmannian manifold so that the operator defined on $R^3 - \{0\}$ is essentially self-adjoint.

In spite of the richness of the mathematics it has produced weak contact of two particles has severe limitations in the physical applications.

This is not the case for weak contact of two particles in a three-particle system (the difference is that the position of the barycenter of the two-particle subsystem cannot be fixed).

In this case there is a self-adjoint extension which has a bound state.

One can also consider *simultaneous* weak contact of three particles. In this case the extension has an Efimov spectrum.

We will discuss this case when we will analyze the Bose gas in the high-density regime.

We shall consider first the case of two particles in weak contact.

Now the [2] boundary conditions require that functions in the domain take a finite value at the boundary.

In the study of weak contact, we can proceed as in the case of strong contact and introduce the Minlos space.

The Krein map is induced again by the operator $(H_0 + \lambda)^{-\frac{1}{2}}$.

This corresponds to fractioning *but there is no mixing*.

In $\mathcal{M}$ the kinetic energy is represented by the operator $(H_0 + \lambda)^{\frac{1}{2}}$ and the potential has a $log(|x_i - x_j|)$ singularity at the coincidence manifold.

The hamiltonian is covariant under dilation

Due to scale covariance this is the behavior of the wave function also at large distances; this is the origin of the zero-energy resonance.

Inverting the Krein map one has in physical space a weakly closed quadratic form bounded below with a $\frac{1}{|x_i - x_j|}$ behavior *at large distances* and therefore a zero-energy resonance (the Krein map does not alter the long-distance behavior).

It is strongly closed [13] and corresponds to a self-adjoint operator bounded below and with a zero-energy resonance.

The hamiltonian and the Krein map are invariant under rotations. Therefore, one can study separately the irreducible components in the angular momentum sectors.

In each of them the weak contact hamiltonian is the limit in strong resolvent sense of the hamiltonian with the approximation potentials V^ϵ *but in the* $L = 0$ *sector a zero energy resonance must be subtracted away* before on can use compactness to prove the existence of the limit.

This explains why in the case of weak contact of two particles *the approximating potentials must have a zero-energy resonance*.

Remark: The case of a weak interaction *in a two-particle system* is discussed in Albeverio and Hoegh-Krohn [3] using methods of Functional analysis in the case when one of the particles has infinite mass. This particle may be considered as a fixed point (point interaction).

The presence of a zero-energy resonance implies a singularity of the resolvent at zero momentum and this requires an accurate and difficult estimate of the zero-energy limit in the B.K.S. formula for the difference of two resolvents [3].

In Albeverio and Hoegh-Krohn [3], this analysis is presented for the weak contact interaction of a particle with a fixed point (a particle of infinite mass) but the same analysis can be done for the case of weak contact interaction of two particles in the reference frame of the barycenter.

12. A PARTICLE IN WEAK CONTACT WITH A PAIR OF IDENTICAL PARTICLES

Consider now the case of a particle *in weak contact* with a pair of identical particles.

We use the same Krein map as the case of strong contact. Therefore, it corresponds to fragmenting the wave functions and in mixing the two channels.

Again, we restrict attention to product states.

The Krein map is mixing and fractioning.

In Minlos space the boundary potentials are represented by a function that has a logarithmic singularity at coincidence hyperplanes (the derivative in polar coordinates has a $\frac{1}{|x_i - x_j|}$ singularity).

The boundary potential and the kinetic energy transform covariantly under dilation.

Therefore, the boundary potential in Minlos space behaves *also at infinity* as $log(|x_i - x_j|)$.

The kinetic energy is still represented by $\sqrt{H_0 + \lambda}$.

Lifting to physical space one has a unique a three-body operator. In the B.K.S. formula for the difference between the resolvent of weak contact and the free resolvent, at the origin in momentum space one has the inverse of a two-by-two matrix with zero on the diagonal.

The matrix is therefore invertible and has a negative eigenvalue (one may say that the two zero energy resonances conspire to give a bound state).

Therefore, if the potential of the weak contact is strong enough *the system has a bound state and no zero energy resonances*.

The same occurs for the sequence of approximating potentials with a zero-energy resonance.

Since there is no zero energy resonance in the difference, the sequence in physical space of the difference the quadratic of the weak contact and that form associated to the potentials V^ϵ is compact in bounded sets in the Sobolev topology it converges to zero when $\epsilon \to 0$.

It has a (Palais.Smale) limit that represents

Proposition 1: A particle *in weak contact* with a pair of identical particles is represented by a self-adjoint operator with one bound state *and no zero energy resonances*.

It is the limit of the hamiltonians with potential V^ϵ that scale as $V^\epsilon(x) = \frac{1}{\epsilon^2} V(\frac{|x|}{\epsilon})$.

There may zero energy resonances due to additional regular potentials, but we shall prove that their contribution is independent of that of weak contact.

A direct study "in physical space" of the limit is not difficult. We sketch some details (based on an unpublished manuscript with A. Michelangeli).

From the analysis of B.K.S it follows that the resolvent $R(z) = \frac{1}{H+z}$ of H satisfies

$$R(z) - R_0(z) = [R_0(z)A_\epsilon^*](1 - Q_\epsilon z))^{-1}[A_\epsilon R_0(z)] \tag{11}$$

$$A_\epsilon = \sqrt{V_1^\epsilon + V_2^\epsilon} \quad Q_\epsilon(z) = A_\epsilon \frac{1}{R_0}(z) A_\epsilon^* \quad R_0(z) = H_0 - \epsilon z \tag{12}$$

If V_1 and V_2 are of class C^1, under the scaling $V \to V^\epsilon(x) = \epsilon^{-2}V(\frac{x}{\epsilon})$ one has

$$lim_{\epsilon\to 0}[\sqrt{V_1^\epsilon(y_1)+V_2^\epsilon(y_2)}-\sqrt{V_1^\epsilon(y_1)}-\sqrt{V_2^\epsilon(y_2)}]=0 \quad (13)$$

and therefore the "overlap" vanishes when $\epsilon \to 0$ and one can substitute $A = \sqrt{V^\epsilon(y_1)}+\sqrt{V^\epsilon(y_2)}$.

Since A_ϵ is the sum of two terms, one has four summands.

To estimate the limit $\epsilon \to 0$ perform *in the integral over internal variables* a scaling $x \to \epsilon^{\frac{3}{2}}x$.

The two integrations implicit in the right-hand side of (12) provide a factor ϵ^3; the product of the two potential provide a factor ϵ^{-4}.

Therefore, to find the limit one can neglect all contributions that are of order >1 in ϵ.

To first order in ϵ there is only a separate contributions of the zero energy resonances in each channel.

This is an invertible two-by-two symmetric matrix with zero on the diagonal. It has therefore a negative eigenvalues.

Substitution in the B.K.S. formula for the difference of two resolvents this produces a bound state if the potential is strong enough and ϵ is sufficiently small.

The limit $\epsilon \to 0$ is the resolvent of the hamiltonian of the system made of a particle of mass 1 in weak contact interaction with two identical bosons of mass one.

Remark 1: The scaling $x \to \epsilon^{\frac{3}{2}}x$ that enters in the rescaling *of the integral over the internal variables* transforms weak contact interaction into strong contact.

We shall come back to this point when we will discuss the Bose-Einstein gas in the high-density case.

Remark 2: The result does not depend on the masses of the particles provided that they are not all zero.

If two of the particles have zero mass the bound state is the Polaron [23]; we will consider this case in detail in **Appendix 1**.

If two of the particles have infinite mass the system represents weak contact interaction with two fixed point (point interaction with two fixed points).

This system has zero energy resonances and therefore the Wave operator is a bounded map $L^p \to L^q$ for $1 < p \leq q < \infty$.

13. THREE PARTICLES IN PAIRWISE WEAK CONTACT: LOW DENSITY BOSE-EINSTEIN CONDENSATE

The Bose-Einstein condensate is a relatively dilute gas of identical bosons in weal contact.

The density is such that the probability to find a third particle nearby is negligible.

Still, due to the zero-energy resonance, (a long-range effect) the presence of a third particle is essential (the particle we consider has a weak contact with *two particles*).

We have seen in the preceding section there is a bound state.

We shall call Ω_w this bound state.

Weak contact is the limit of an attractive potentials of very short radius ϵ and a zero-energy resonance.

If ϵ is very small *and if the gas is diluted* one can choose $\epsilon^{-1} = N$ and regard the subsystems as composed of only three particles in weak contact. The bound state Ω_w is stable because the hamiltonian of the two-particle subsystem is positive (and have a zero-energy resonance).

A zero energy (Fesbach) resonance is required for the interaction of the two-body pairs. Once formed, the pairs are stable.

Since the gas is very diluted the probability that *all three particles are very close* is negligible (notice the interaction has range ϵ).

But the particles are identical and satisfy Bose-Einstein statistics.

Their state is therefore "entangled," and each pair has equal probability to be in weak contact.

Since the particles are identical, *it is as if* the system be composed of separate pairs of particles.

The ground state of the system of $2N$ particles is the tensor product of the vectors $\otimes\Omega_w^i$ for all different two-body pairs (properly symmetrized since the particles are identical bosons).

The error is of order $\frac{1}{N}$.

Since the two (identical) bosons in the pair are in (weak) contact and each of them satisfies the Schrödinger equation with as potential the density of the other, each of two bosons satisfies the Gross-Pitaewskii equation for a Bose-Einstein condensate with an *effective coupling potential* due to the presence of a zero-energy resonance [24].

Remark 1: In Benedikter et al. [25] to have the right scaling one adds an extra N factor (N is the number of particles).

This scaling is justified with the assumption that *each particle contributes for a fraction* $\frac{1}{N}$.

In our approach the correct scaling is a consequence of weak contact.

The probability of having a correlation with a third particle (and therefore with another pair) vanishes as ϵ and this is the basis for the proof of condensation in Khowles and Pickl [26]. Since weak contact is limit of a potential with very short range $\frac{1}{N}$ and the gas is very diluted the error term in neglecting the interaction with the other pairs is proportional to $\frac{1}{N}$ and one can use perturbation theory to describe the interaction between pairs.

To first order the ground state is a collection of non-interacting weakly bound pairs.

Choosing $\epsilon \equiv \frac{1}{N}$ permits a Fock space analysis.

We will not analyze further here this problem .

14. BOSE-EINSTEIN CONDENSATE, THE HIGH-DENSITY CASE, THE NEW GROUND STATE

Consider now the high-density case.

The particles are now *simultaneously* in weak contact.

The interaction s represented, before taking the limit $\epsilon \to 0$ by the hamiltonian

$$H_{int} = H_0 + \sum_{i\neq j\neq k} \frac{1}{\epsilon^2} V(\frac{|x_i - x_j|}{\epsilon}) \tag{14}$$

In Krein space we can use perturbation theory.

In the perturbation formula for the resolvent the terms that depend only on two of the potentials give the same result of the weak contact interaction of one particle with a pair.

We are interested in the contribution of terms *that depend on all three potentials*.

In this contribution we can "artificially" take away two ϵ from the denominator of one of the potential and "give" an ϵ^{-1} factor to each of the other two (this artifice does not alter the result).

The remaining potential now plays no role.

Redistributing the ϵ is an artifice but it leads to the conclusion that at high density *the ground state of system* is better described considering a system of three particles one of which is in *strong* contact with the other two.

The strong contact interaction takes place *separately* with the two particles; since the particles are identical one has a gas two particles strongly bound.

Remark that the presence of a third particle is mandatory to define strong contact. The role of the third particle is to prevent free motion for the barycenter of the two particles in strong contact.

Call Ω_s the ground state. To first order the ground state of the high-density Bose-Einstein gas is $\otimes_i \Omega_s^i$.

It is not related to the ground state $\otimes_i \Omega_w^i$ of the diluted Bose-Einstein gas.

Since the two (identical) bosons in the pair are in strong contact, each of them satisfies the Schrödinger equation with as potential the density of the other i.e., the focusing cubic Schrödinger equation (and not the Gross-Pitaewskii equation which has *a different effective coupling constant* due to the presence of a zero energy resonance) [24].

15. EFIMOV EFFECT IN QUANTUM MECHANICS

The Efimov effect in Quantum Mechanics is the presence of an Efimov sequence of bound states for a particle that moves in a potential that is the sum of two potentials which taken separately have a zero-energy resonance.

In spite of the same name, the effects have *totally different origin*.

They lead to the same result because in the two cases there is the same balance of kinetic and potentials energies.

We assign +2 for each of the three particles particle (since they satisfy a second order differential equation) and –3 two strong contacts (the power of ϵ^{-1} in the scaling). If the difference is zero one has Efimov spectrum.

In the quantum mechanical case there is only one second order differential operator and there are two weak contacts with two resonances; for the counting of weights this is the same as a weak contact with the resulting bound state.

One assigns - 2 to weak contact with bound state. The net sum is zero as in the three-particle case with strong contact.

Therefore, one can expect to have the same effect (this counting is not a substitute for proofs but, in spite of its empirical flavor, provides very efficient indications).

A proof of the Efimov effect in Quantum Mechanics for contact interactions can be obtained using the Krein map.

The Krein map is well defined.

Setting equal to one the mass of the particle in Minlos space the kinetic term is $\sqrt{-\frac{1}{2}\Delta + \lambda}$.

The two zero energy resonances conspire to a give a bound state and this gives a negative quadratic form with a singularity of degree –1 at the origin in position space.

This leads to a Weyl limit circle singularity as in the three particles case.

Inverting the Krein map and making use of Gamma convergence one obtains the Efimov spectrum as in the three-particle case.

Remark: Notice that we have used only the existence of two zero energy resonances and the fact that the Schr odinger equation is of second order; therefore, this analysis through the Krein map applies as well to the case of smooth potentials, leading to an alternative proof usual Efimov effect in QM [27, 28].

In the same way one can analyze the case of the Pauli equation for non-relativistic spinors.

The Pauli equation is a first order differential equation (for spinors) with positive generator.

In one dimension one can use as contact potential the delta function; this gives a contact of weak type at the vertex for a system of three particles that move on a Y-shaped graph and interact at the vertex.

There is a bound state since there are three operators and only two weak contacts (in one dimension the delta function represents a weak contact interaction because it scales as the differential operator).

At the end we shall return briefly to this system.

16. STRONG AND WEAK CONTACT ARE INDEPENDENT

Theorem 2: In three dimensions for $N \geq 3$ contact interactions and weak-contact interactions contribute *separately* and *independently* to the spectral properties and to the boundary conditions at the contact manifold.

Contact interaction contribute to the Efimov part of the spectrum and to the T-M boundary condition $\frac{c_{i,j}}{|x_j - x_i|}$ at the boundary $\Gamma \equiv \cup_{i,j} \Gamma_{i,j}$.

Weak-contact interactions contribute to the constant terms at the boundary and may contribute to the (finite) negative part spectrum. ◇

Remark: This theorem states that all results of the weak-contact case (in particular for point interactions) remain valid when strong contact interactions are added.

Proof. For an unified presentation (which includes also the proof that the addition of a regular potential does not change the picture) it is convenient to use a symmetric presentation due to Konno and Kuroda [4] (who generalize previous work by Krein and Birman) for hamiltonians that can be written in the form

$$H = H_0 + H_{int} \qquad H_{int} = B^* A \tag{15}$$

where B, A are densely defined closed operators with $D(A) \cap D(B) \subset D(H_0)$ and such that, for every z in the resolvent set of H_0, the operator $A\frac{1}{H_0+z}B^*$ has a bounded extension, denoted by $Q(z)$. We give details in the case $N = 3$.

Since we consider the case of attractive forces, and therefore negative potentials it is convenient to denote by $-V_k(|y|)$ the two body potentials.

The particle's coordinates are $x_k \in R^3, k = 1, 2, 3$.

We take the interaction potential to be of class C^1 and set

$$V^\epsilon(X) = \sum_{i\neq j}[V_1^\epsilon(|x_i - x_j|) + V_2^\epsilon(|x_i - x_j|) \tag{16}$$

where V_1 and V_2 are negative and $V_3(|y)$ is a regular potential.

For each pair of indices i, j we define $V_1^\epsilon(|y|)) = \frac{1}{\epsilon^3}V_1(\frac{|y|}{\epsilon})$ and $V_2^\epsilon(|y|) = \frac{1}{\epsilon^2}V_2(\frac{|y|}{\epsilon})$.

The limit corresponds, respectively to contact and weak-contact.

We define $B^\epsilon = A^\epsilon = \sqrt{-V^\epsilon}$.

For $\epsilon > 0$ using Krein resolvent formula one can give explicitly the operator B^ϵ as *convergent power series* of products of the free resolvent $R_0(z), Rez > 0$ and the square roots of the sum of potentials $V_k^\epsilon \;\; k = 1, 2, 3$. One has then for the resolvent $R(z) \equiv \frac{1}{H+z}$ the following form [4]

$$R(z)-R_0(z) = [R_0(z)B^\epsilon][1-Q^\epsilon(z)]^{-1}[B^\epsilon R_0(z)] \qquad z > 0 \tag{17}$$

with

$$R_0(z) = \frac{1}{H_0 + z} \qquad Q^\epsilon(z) = B^\epsilon \frac{1}{H_0 + z} B^\epsilon \tag{18}$$

If $\epsilon > 0$ the Born series converges and the resolvent can be cast in the Konno-Kuroda form [4], where the operator B is given as (convergent) power series of convolutions of the potential U^ϵ and V_1^ϵ with the resolvent of H_0.

In general

$$\sqrt{V_1^\epsilon(|y|) + U^\epsilon(|y|)} \neq \sqrt{V_1^\epsilon(|y|)} + \sqrt{U^\epsilon(|y|)} \tag{19}$$

and in the Konno-Kuroda formula for the resolvent of the operator H_ϵ one loses separation between the two potentials V_1^ϵ and U^ϵ.

Notice however that, if V_1^ϵ and U^ϵ are of class C^1 , the L^1 norm of U^ϵ vanishes as $\epsilon \to 0$ uniformly on the support of V_1^ϵ.

By the Cauchy inequality one has

$$lim_{\epsilon\to 0}\|\sqrt{V_1^\epsilon(y)}.\sqrt{U^\epsilon(y)}\|^1 = 0 \tag{20}$$

Therefore, if the limit exists the strong and weak contact interactions act independently.

In the same way one proves the independence of the strong and weak contact interactions from the regular interaction.

The weak-contact part has a limit in strong resolvent sense.

The limit is unconditional, i.e., it does not depend on the particular denumerable subsequence $\epsilon_n \to 0$ used.

The strong contact part has a limit along minimizing sequences by Theorem 1.

Therefore, the joint limit exits along these minimizing sequences. ♡

17. WEAK-CONTACT CASE: SEPARATION OF THE REGULAR PART

Consider now *separate* weak-contact interaction of a particle with a pair of identical particles.

We allow for the presence of a "regular part" represented by a smooth two body L^1 potential of finite range and call *singular part* the quasi contact interaction and the resonance.

Theorem 3: For a weak-contact interactions the singular term (pure weak-contact) and the regular term in the two-body part of the interaction *contribute separately* to the spectral structure of the hamiltonian. ◇

Proof. For the proof we use again the Konno-Kuroda resolvent formula but now for a system with potentials $V_2^\epsilon + V_3$.

Recall that set $V_2^\epsilon(|x|) = \frac{1}{\epsilon^2}V_2(\frac{|x|}{\epsilon})$.

The Konno-Kuroda formula is now for $Re(z) > 0$ and $R_0^\epsilon(z) = H_0 + \epsilon z$

$$\frac{1}{H_\epsilon + z} - \frac{1}{H_0 + z} = -\frac{1}{H_0 + z}Q^\epsilon B^\epsilon Q^\epsilon \frac{1}{H_0 + z} \tag{21}$$

$$B^\epsilon = \sqrt{V_2^\epsilon + V_3} \quad Q^\epsilon(z) = B^\epsilon \frac{1}{R_0}(z)B^\epsilon \quad R_0(z) = (H_0 + \epsilon z)^{-1} \tag{22}$$

One can now repeat the procedure in Theorem 3.

By assumption V_2 and V_3 are of class C^1 and as $\epsilon \to 0$ on the support of V_2^ϵ the L^2 norm of V^3 is of order ϵ.

Therefore

$$\|(\sqrt{V_3^\epsilon} + \sqrt{V_2^\epsilon})^2 - V_3^\epsilon - V_2^\epsilon\| = 0(\epsilon) \tag{23}$$

We conclude that in limit the potentials V_2 and V_3 contribute *additively* to spectral properties.

The potential V_2 (weak-contact) may contribute for a finite or infinite number of elements of the spectrum (depending on the masses and the coupling constants), the potential V_3 gives a contribution to the spectral measure.

In both case there are no singularities at the bottom of the (absolutely) continuous spectrum.

This proves Theorem 3. ♡

Remark: The zero-energy resonance we have found *is due to a very sort range potential* (in the limit, zero range) whereas the possible resonances of the regular potentials are due *to their very long range*.

The presence of one does not interfere with the presence of the other.

18. CONNECTION WITH OTHER APPROACHES

Heat kernel renormalization

We comment briefly on the relation with the "heat kernel" renormalization introduced in Erman and Turgut [29].

Start with the identity

$$\int_0^\tau e^{-H_0+\lambda}dt = \tau + \frac{1}{H_0+\lambda} + O(\frac{1}{\tau}) \tag{24}$$

where H_0 is the free hamiltonian.

The heat kernel renormalization consists by definition in taking the limit $\tau \to \infty$ and neglecting the divergent constant.

Since $H_0 + \lambda$ commutes (formally) with a delta distribution (a constant in Fourier space) the heat kernel renormalization of the potential V^ϵ for the three-body system

$$V^\epsilon \to \frac{1}{\sqrt{H_0-\lambda}} V^\epsilon \frac{1}{\sqrt{H_0+\lambda}} \tag{25}$$

may be defined as a regularization map for $\epsilon > 0$ and in the limit $\epsilon \to 0$ is the interaction potential in $\mathcal{M}$.

Recall that the Krein map is a "fractioning" of the "wave function" (the wave function becomes more singular) *while switching the channels* which results in mixing.

In this case this "renormalization" consists in using Gamma convergence after the inversion of the Krein map (i.e., in physical space).

This is clearly a non-perturbative scheme and does not require "removing infinities."

We recall that Gamma-convergence is equivalent to resolvent convergence i.e., roughly speaking, convergence under the assumption that one considers sequences of states on which the hamiltonian stays bounded (this is the role of renormalization).

Interior boundary conditions

This approach has been proposed recently, mostly in view of a second-quantization scheme [20, 30, 31].

With different wording and different analytical techniques this approach has some similarities with the one which is developed here.

After all, the boundary conditions at the contact manifold are "interior boundary conditions."

In an **Appendix** we develop a second quantization scheme (similar to that in Lampart [30]) adapted to the self-adjoint extensions discussed here.

It is a "baby second quantization scheme," adapted to the three-body contact interaction for one massive and two massless particles, in which only the zero mass particles undergo second quantization.

Notice that a quantum mechanical three body problem arises naturally if creation and annihilation operators are "partially dequantized" by choosing for *two of the zero mass particles* the ground state of a system in which the zero mass particles are in strong contact interaction with the massive one.

The ground state of the system is then obtained choosing for the remaining particles the vacuum state of a suitable representation of the c.c.r.

The resulting ground state is a model for the *polaron* [32], the ground state of the Nelson model [23]. We discuss this model in the **Appendix**. We can also in the same way find the excited states below the continuum by choosing different bound states of the three-body problem and the vacuum of another suitable representation.

Changing the bound state changes also the representation.

Notice that this procedure limits the role of strong contact interaction in quantization problems to *linear couplings* of a particle and a quantized field.

19. DETAILS FOR SOME SIGNIFICANT CASES IN THREE DIMENSIONS

We study in the following systems of non-relativistic bosons and fermions that satisfy the Schrödinger equation.

Later we will consider on a lattice electrons which are fermions and satisfy the Pauli equation.

Since the Pauli equation is a first order differential equation, weak contact plays the same role as strong contact in the bosonic case.

For boson we shall discuss in what follow, both for strong and weak contact , some relevant case; they are sufficient to draw conclusions on a system of an arbitrary number of particles.

In particular we shall consider in three dimensions

I) A particle of mass m in strong or weak contact interaction with two identical bosons of unit mass.
II) A particle of mass 1 in strong contact with two fermions of the same mass.
III) Two pairs of identical bosons in strong contact whose barycenters are in weak contact
IV) The same problem for fermions,
V) N pairs of boson or fermions in strong contact.

In the case of strong contact for fermions we prove that the hamiltonian *is positive for any value of N*. This system is called *Unitary gas*.

In the case of bosons, the (negative) lower bound of the spectrum is linear in N.

I

Consider first the case of a particle of mass m in strong contact interaction with two identical bosons of unit mass.

Setting again for simplicity $\lambda = 0$ the quadratic form in $\mathcal{M}$ is the sum of two terms

$$Q = Q_1 + Q_2 \tag{26}$$

where

$$Q_1(\phi) = \frac{m}{m+1}(\phi, \sqrt{H_0}\phi) \tag{27}$$

while the kernel of Q_2 is

$$Q_2(p,q) = -\frac{\frac{2}{1+m}(p.q)}{(p^2+q^2)^- \frac{1}{(1+m)}(p.q)} \tag{28}$$

Again, this kernel quadratic reaches its minimum value at $q = p$.

In Fourier transform one has

$$B(m)\sqrt{-\Delta} - D(m)\frac{1}{|x|} + \Xi"(m) \tag{29}$$

where $B(m), D(m)$ are suitable positive functions of the parameter m and Ξ'' is a positive form with a smooth kernel that vanishes on the diagonal.

We consider only the case $\Xi = 0$. The contribution of Ξ is small and does not alter the conclusions.

Following Derezinky and Richard [14] proves that for each eigenvalue l of the angular momentum there are threshold N_l^*, N_l^{**} such that for $m > N_l^{**}$ the spectrum is absolutely continuous and positive.

For $N_l^* < m \leq N_l^{**}$ there is a continuous family of self-adjoint extensions, each with a negative eigenvalue, and for $0 < m \leq N_l^*$ the negative spectrum is pure point and accumulates geometrically to $-\infty$ (a Weyl limit circle effect).

One can verify that for equal masses $N_0^{**} > 1$ while $N_l^* < 1$ for all $l \geq 1$.

Therefore, in the equal mass case there is a family of extensions; for each of them there is a family of bound states with energies that diverge linearly to $-\infty$.

Inverting the Krein map by Gamma convergence one has

Proposition 2: The hamiltonian of a pair identical bosons in strong contact interaction with a third particle of the same mass has an Efimov sequence of bound states if the interaction is strong enough. The support of the wave functions is larger for decreasing energy; the wave functions belong to the form domain. ◇

II

We consider next in R^3 the case of a particle of mass m in strong contact with a pair of fermions with the same mass.

The analysis proceeds as in the strong contact case but since the contact is weak the integral in the integrand in Q_2 must be anti-symmetrized.

Now one has

$$(\phi, Q_1\phi) = \frac{m}{m+1}(\phi, \sqrt{H_0 + \lambda}\phi) \tag{30}$$

while the kernel of Q_2 is

$$Q_2(p,q) = \frac{2}{1+m}\frac{1}{|p-q|^2}(p^2+q^2)^2 - \frac{4}{(1+m)^2(p.q)^2} \tag{31}$$

These are the quadratic forms in $\mathcal{M}$ that correspond, respectively the kinetic energy and to the distributional potential.

For the study of spectral properties, it is convenient to notice that the kernel of Q_2 is positive (it has a positive maximum at $p = q$).

Since the Krein map is positivity preserving in physical space the operator is positive.

Proposition 3: *The hamiltonian of a pair of fermions of mass m which are in strong contact with a third particle of the same mass has a positive spectrum.* ◇

20. III, STRONG AND WEAK CONTACT IN A FOUR BOSONS SYSTEM

We have analyzed the case of three particles.

Consider now a four bosons system. We assume that there is a strong contact of any particle with two other particles ad in addition there is a weak contact between the barycenters of any two pairs.

Notice that the total degree of the kinetic terms is eight (two for each particle) and the total degree of the interaction term is also eight (three for each strong contact and two for the weak contact).

Therefore, we expect to have an Efimov sequence of four-bound states (quadrimers).

The analysis is simple in momentum space.

The explicit expressions of these forms in momentum space were known to R.Minlos (private communication).

We choose as coordinates the difference of the coordinates of the particles in strong contact and the difference of the coordinates of the barycenters.

The strong interactions within a triple gives a contribution that we have already analyzed.

The only difference is the presence of the weak interaction between the barycenters. In Minlos space the kinetic energy is represented by $\sqrt{H_0 + \lambda}$.

The interaction is the sum of three terms C_i, $i = 1, 2, 3$.

C_1 and C_2 are the images in $\mathcal{M}$ of the convolution of the four-particle Green function with the strong interaction potentials.

$$\begin{aligned}(\phi, C_1\phi) &= (\phi, C_2\phi) \\ &= \int dkdsdw\bar{\phi}(k,w)\frac{\phi(s,w)+\phi(k,s)}{k^2+s^2+w^2+(k,s)+(k,w)+(s,w)}\end{aligned} \tag{32}$$

Contributions C_1, C_2 refer to the three-particle case, i.e., a particle in strong contact with two other particles.

It is different from the case of three particles we have considered before because of the presence of a fourth particle.

The presence of a fourth particle is irrelevant because it only enters the definition of the Krein map, which is inverted at the end.

C_3 is a genuine four particle term which is not present in the three-particle sector. It describes the (weak) interaction of the two barycenters.

The corresponding quadratic form in M is

$$(\phi, C_3\phi) = -\int dwdsdk \frac{\bar{\phi}(k,s)\phi(w-\frac{k+s}{2}, -w-\frac{k+s}{2})}{w^2+\frac{3}{4}(k^2+s^2)+\frac{1}{2}(k,s)} \quad (33)$$

(this quadratic form was known to R. Minlos, private communication).

The form has a simpler structure when written as a function of the difference of coordinates of the barycenters of the two pairs. In these coordinates it is the image *in the four-particle sector* of an "effective" weak contact interaction between the barycenters of the two pairs. Weak contact between the two barycenters gives a system with at most a finite number of bound states.

Therefore, in Krein space the system is described by a two-parameters family of operators which have an infinite number of bound states with eigenvalues that diverge linearly to ∞ and a self-adjoint operator wit at most a finite number of bound states.

Inverting the Krein map one obtains a two parameter families of weakly closed forms.

By construction, the form is invariant under rotation but also under permutation of the particles.

We decompose again in irreducible representation of the rotation group and quotient it by the permutation group.

Each component is now strictly convex, and we can use Gamma convergence to extract a convergent subsequence.

This give a unique weakly closed quadratic form bounded below that can be closed strongly and provides a self-adjoint operator with an Efimov spectrum.

Since it is a four-body system it describes an Efimov sequence of *quaternions*.

Therefore

Proposition 4: *If the interaction is strong enough a system of two pairs of bosons in strong contact and with a weak contact between the barycenter has an Efimov sequence of quaternions.* ◇

Four-body Efimov states have been reported experimentally [16, 21].

21. IV. THE CASE OF FERMIONS

Consider the system of two pairs of identical spin $\frac{1}{2}$ fermions of mass one which satisfy the Schrödinger equation and in contact interaction. Spin $\frac{1}{2}$ is required because antisymmetry of the wave functions of parallel spins is zero at contact. The generalization to N identical spin $\frac{1}{2}$ fermions will describe the unitary gas.

In $\mathcal{M}$ the quadratic form of the system is the sum a term C_0 which represents the kinetic part of form minus three forms $C_1,\ C_2\ C_3$.

The explicit expressions of these forms in momentum space were known to R.Minlos (private communication).

C_1 and C_2 are the images in $\mathcal{M}$ of the convolution of the four-particle Green function with two delta singularities of the potential between two fermions with opposite spin.

$$\begin{aligned}(\phi, C_1\phi) &= (\phi, C_2\phi)\\ &= \int dkdsdw\bar{\phi}(k,w)\frac{\phi(s,w)+\phi(k,s)}{k^2+s^2+w^2+(k,s)+(k,w)+(s,w)}\end{aligned} \quad (34)$$

As in the tree particles case, when written in space coordinates they have a Coulomb type singularity in different variables related to the possible triples. But now due to antisymmetry the coefficient of the Coulomb term is positive.

C_3 is a genuine four particle term which is not present in the three-particle sector.

It represents an effective interaction between the barycenters of the two pairs.

Notice that a pair of fermions with opposite spin has the symmetry a boson.

The corresponding quadratic form in M is

$$(\phi, C_3\phi) = -\int dwdsdk \frac{\bar{\phi}(k,s)\phi(w-\frac{k+s}{2}, -w-\frac{k+s}{2})}{w^2+\frac{3}{4}(k^2+s^2)+\frac{1}{2}(k,s)} \quad (35)$$

It has a simpler expression when written as a function of the difference of coordinates of the barycenters of the two pairs. In these coordinates it is the image *in the four-particle sector of* $\mathcal{M}$ of an "effective" contact interaction between the barycenters of two pairs with opposite spin. Notice that only *pairs of particles* enter this term.

The form can be decomposed into a symmetric and antisymmetric part under interchange *of the two pairs*.

Only the kinetic energy contributes to the antisymmetric part; this part is positive.

Also, the symmetric term of is positive.

Therefore, the quadratic form is positive.

Since the Krein map is positivity preserving the same is true in physical space and the system is described by a positive hamiltonian (with a zero-energy bound state).

Proposition 5: *The operator associated to a system two pairs of identical fermions in strong contact and such that the barycenters are in weak contact is a positive self-adjoint operator in* $L^2(R^{12})$. *Its hamiltonian is the limit, in the strong resolvent sense, of a sequence of approximating hamiltonians with potentials of decreasing support.* ◇

Remark: In Michelamgeli and Pfeiffer [33], positivity of the spectrum was conjectured with the aid of a computer.

V: the case of N particles. We have considered so far the cases $N = 3$ and $N = 4$.

Consider now the case of N identical bosons.

For N particles the negative part of the spectrum is *entirely due either to a strong contact of tree bodies or to the four-body contact described in Proposition 4.*

Therefore

Proposition 6: The energy of a gas of N bosons in strong contact interaction is bounded below by $-CN$ which the positive constant C depends on the strength of the interactions.

The system described by any number of identical fermions in weak or strong interaction is described by a positive hamiltonian. This system is often call often called *Unitary gas.* ◇

22. TWO DIMENSIONS; SIMULTANEOUS PAIRWISE WEAK CONTACT

In the two-dimensional case strong contact interaction is a distributional potential $\delta(|x_i - x_j|)$ at the coincidence manifold.

It is the limit of the interaction through two-body potentials of that scale as $V^\epsilon(|y|) = \frac{1}{\epsilon^2} V(\frac{|y|}{\epsilon})$.

The Krein map is the same as in three-dimensional case.

Again, in Minlos space the free hamiltonian H_0 is represented by $(H_0 + \lambda)^{\frac{1}{2}}$ and the potentials differ from $-\frac{C}{|x_i x_j|}$ for a smooth positive quadratic form.

One has therefore

Propostion 7: *In two dimensions strong simultaneous pairwise weak contact interaction of three bosons is represented by the potential* $-C\sum \delta(|x_i - x_k|), \quad C > 0$.

It is well defined in physical space through Gamma convergence. It is the limit for $\epsilon \to 0$ *of potentials that scale as* $V^\epsilon(|x|) = \frac{1}{\epsilon^2} V(\frac{|x|}{\epsilon})$

The system has an Efimov sequence of bound states. ◇

Since there are no zero energy resonances the mapping properties of the Wave operator in physical space are $L^p \to L^q$ for $1 < p \leq q < \infty$.

This result has been obtained also for regular potentials in Erdogan et al. [34]).

23. TWO DIMENSIONS, SEPARATE STRONG CONTACT

Consider now a system of three identical bosons in which each has a strong contact with the other two.

We describe in detail the hamiltonian of the resulting system.

To study the structure of the operator we study its quadratic form and assume a before that the particles are *identical bosons*. The wave function in the frame of reference of the barycenter is best written as a function of one radial coordinate r and two Euler coordinates on S^3.

We define $r^2 = (|x_1 - x_3|)^2 + (|x_2 - x_3|)^2 \quad x_k \in R^2, \quad r \in R^+$.

In the Theoretical Physics literature this coordinates are called "homogeneous."

The quadratic forms we consider have the same structure as in the case of three dimensions but in two dimension the singularities are different.

Again, we use a Krein map with the compact operator $\sqrt{H_0 + \lambda}^{-\frac{1}{2}}$ (for each particle there are two contacts).

For simplicity we take $\lambda = 0$ in the following formulae.

If we denote by $x_k \in R^2 \quad k = 1, 2, 3$ the coordinates of the three points with $x_1 + x_2 + x_0 = 0$ one has in $\mathcal{M}$ for the quadratic forms

$$Q(\phi) = Q_0(\phi) + Q_1(\phi) \tag{36}$$

where

$$Q_0 = (\phi, \sqrt{H_0 + \lambda})\phi) \tag{37}$$

In the center of mass, using Fourier coordinates conjugated with $x_1 - x_3$ and $x_2 - x_3$, the *kernel* of Q_1 is

$$\frac{1}{(q_1^2 + q_2^2 + (q_1, q_2) + \lambda)(q_1 + q_2)^2 + \lambda} \qquad q_i \in R^2 \tag{38}$$

Setting

$$(x_1 - x_3)^2 + (x_2 - x_3)^2 = r^2 \quad r \in R^+ \tag{39}$$

the kernel Q_1 can be written in spatial homogeneous coordinates as integral over S^3 of a kernel $-C\frac{1}{r} + W(x_1, x_2, \lambda)$ where $C > 0$ and W is a smooth kernel which vanished in the diagonal.

On now proceeds as in the three-body case in R^3 with weak contact interactions.

Proposition 8: In two dimensions the pairwise strong contact of three identical bosons is represented by a hamiltonian which, if the interaction is strong enough, has a bound state.

Since there are no zero energy resonances the Wave Operator for the system is a bounded map from L^p *to* L^p *for all* $1 < p < \infty$. ◇

24. ONE DIMENSION. LATTICE STRUCTURE. THE FERMI SEA

The purpose of the following section is manly to have a rough picture of the Fermi sea.

We follow the usual description according to which nuclear forces the *conduction electrons* to move on a graph-like stricture with Y-shaped vertices.

The nucleus can be considered fixed at the center of the cell have a weak contact with the two inner electrons (weak contact at a larger scale is Coulomb interaction).

The system has therefore a bound state of energy $-K$ and the two internal electrons have a wave function (essentially) localized at the center of the cell.

Conduction electrons move on the graph and satisfy the Pauli equation (a first order differential equation for a two-component spinor).

The generator is the (positive) Pauli operator

$$P \equiv i\sigma.\nabla + mI, \quad m > 0 \tag{40}$$

(σ_i are the Pauli matrices and I is the unit matrix).

Notice that the structure of the graph is entirely due to the position of the nuclei. The vertices are Y-shaped.

The interaction of the conduction electrons on the lattice takes place at the vertices.

The lattice stricture forces the conduction electrons to change direction at the vertices; before and after the vertex the conduction electrons *are closer to the nucleus*.

This can be represented by a (negative) potential. The kinetic energy is not changed; in this sense the interaction is attractive.

We describe it by a weak contact at the vertex and therefore there is a zero-energy resonance.

Since there are two electrons moving on the lattice this gives a bound state.

Since the momentum is discontinuous at the vertex the interaction depends on both position a momentum.

We represent this by allowing the (negative) energy of this bound state to be in an interval $[-c, 0)$.

In an extended crystal by the Pauli exclusion principle all these states are occupied: *this is the Fermi sea*.

The electrons "near the surface" have negligible energy. The wave functions are essentially flat, and they have "a Dirac spectrum."

In presence of an electric field along the edge, since the electrons are charged particles, a flow of current is generated. Spins at the two ends of an edge form a magnetic dipole; in presence of a magnetic field the orientation of the dipole is changed.

At the semiclassical scale one can introduce smooth magnetic fields (in the previous scale they correspond to discontinuous potentials); at this scale the motion of electrons *on the surface of the Fermi sea* is seen as classical motion of point particles which satisfy the laws of *classical* electrodynamics [35]. The formalism we have described leaves room also to the "magnetic" Pauli operator.

Of course, at the semiclassical level in presence of electromagnetic fields the Fermi surface can have a complicated structure and the description of dynamics of a point on the Fermi surface may require a refined analysis [35].

AUTHOR CONTRIBUTIONS

The author confirms being the sole contributor of this work and has approved it for publication.

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APPENDIX 1

A. THE POLARON

We treat the Polaron problem ([N][G][FS]) in the context of second quantizaton.

Second quantization can be thought as Weyl quantization for a system with an infinite number of particles.

Lebesgue measure is substituted by a measure on function space (Gauss measure in the Bose case).

Functions on phase space can be represented by the coefficients of their Fourier transforms.

Very roughly speaking for bosons in second quantization a wave function f is substituted with of a scalar field $\Psi(f) = a(f) + a^*(\bar{f})$ where $a(f)$ (resp. $a^*(\bar{f})$) destroys (resp. creates) a particle with wave f. Both terms are linear in f.

The field satisfies the (non-relativistic) commutation relations $[\Psi(\bar{f}), \Psi(g)] = (f, g)$.

In the Fock representation one postulates the existence of a vector Ω (the "vacuum") such that $a(f)\Omega = 0\ \forall f$ in the Hilbert space.

Fock space is the space generated by repeated action of the $a^*(f)$ on Ω (this justifies the name "creation operators").

We shall use the formalism of second quantization and denote by $a((k)$ (resp. $a^*(k)$) the annichilation (resp. creation) of a zero mass particle "of momentum k" (we omit the more precise definition).

In the following we consider the contact interaction of the particle of mass m with any two non relativistic zero mass particles in the second quantization formulation for the field.

This system is called *polaronic* and the ground state is the *polaron* [N].

We take the interaction to be weak contact of the massive particle with any two of the zero mass particles.

We approximate the interaction by using the two-body potential $V^\epsilon = \frac{1}{\epsilon^2} V(\frac{|x_i - x|}{\epsilon})$ where $V \in C^1$.

$$H^\epsilon = H_0 + \int V^\epsilon(x - y_1)\Psi(y_1)dy_1 + \int V^\epsilon(x - y_2)\Psi(y_2)dy_2$$
$$H_0 = -\frac{1}{2m}\Delta_x + \int \omega(p)a^*(p)a(p)dp \tag{A1}$$

where $\omega(p) = |p|^2$ and the $a(k)$ satisfy the c.c.r.

The limit $\epsilon \to 0$ is the contact interaction of the particle with the field.

We have proved that this system has a bound state Ψ. We denote by $\hat{H}$ the hamiltonian.

We use the formalism of second quantization *paying attention* to the fact that for zero mass particles there infinitely *inequivalent* representations of the c.c.r.

A vector of finite energy in the Hilbert space may contain an infinity of zero mass particles with smaller and smaller momentum (this is known as *infrared problem*).

We denote by H the limit hamiltonian. It describes the contact interaction of the massive particle with the cloud of zero mass particles.

To find the structure of the ground state (the Polaron) we will "partially dequantize" the field by choosing properly the state *of two of the zero mass particles* (and therefore the representation of the c.c.r. since the zero mass particles are identical).

We have previously remarked that the weak contact interaction of a particle of mass m with two particles of zero mass leads to a bound state.

Let $\Phi(x)$ be the wave function.

To find the ground state of the combined system we fiber the second quantization space of the zero mass particles *choosing as parameter the position of the particle of mass m*.

We choose the representation by defining annichilation operators

$$A_x(y) = a(y) - \Phi(x) \tag{A2}$$

For each value of x the (distribution valued) operators $A_x(y)$ satisfies the same c.c.r as the operators $a(y)$ but the two representations are *inequivalent*.

Different values of the position of the particle of mass m correspond to a different "infrared behavior" of the mass zero field.

If one writes the Hamiltonian as a function of the field $A_x(y)$ one obtains

$$H = \hat{H} + \int \omega(p)A_x^*(p)A_x(p)dp$$

Remark: In the Theoretical Physics literature this operation goes under the name of "completing the square" and the particle of positive mass is now "dressed" with the a particles

In order to minimize the energy one must choose the Fock representation for A_x for every x. .

The minimum of energy is obtained on the vaccum.

It is convenient therefore to write the relation between A_x and a in the following way

$$a(y) = A_x(y) + \Phi(x) \tag{A3}$$

The self-adjoint operator $\hat{H}$ has a ground state Φ.

There is no coupling.

Therefore, the ground state Ψ of the entire system (i.e., the *polaron*) is at each point x the product $\Phi \times \Omega_x$, where Ω_x is the vacuum in the A_x representation, properly symmetrized. .

By construction the A_x representation is *inequivalent* to the a representation.

The ground state of the system (the polaron) is a "cloud" of *infinitely many* mass zero identical particle with distribution that depends on the wave function $\Omega(x)$.

The cloud *depends on the coordinate of the heavy particle*. [N] [F,S], [L,S], [S].

APPENDIX 2

B. A FIELD THEORY APPROACH

In the following we make some (tentative) comments on a *Field Theory* approach.

In case of the Polaron we have chosen a non relativistic quantization for the Bose field since the particle is non relativistic.

The theory is hybrid since Fock space is used for the mass zero field but not for the particle.

On can place contact interaction in a fully relativistic setting in the context of Relativistic Quantum Field Theory.

Notice that "being in contact at a given time" is a relativistic invariant statement.

Define the Krein map as in the non relativistic case but now with the free relativistic hamiltonian H_{rel} of Relativistic Field Theory (a positive operator *in Fock space*).

The Krein map acts differently on the kinetic part and on the interaction term, *and also this is a relativistic invariant statement*.

Gamma convergence is a minimization procedure, and therefore a relativistic invariant.

The Fock representation is a Gaussian measure space in the case of bosons, Berezin-Segal measure space in the case of fermions.

We consider here only the case of bosons.

In relativistic Fock (r-Fock space) space the free hamiltonian for bosons is $H_0 = \sum_n (-\Delta_n + m_n)^{\frac{1}{2}}$.

In order to have "strong contact" with interaction hamiltonian density formally given by "$\phi^3(x)$" one must use a space in which the hamiltonian is a second order differential operator and therefore one must use a Fock space based on $\mathcal{H}^{-\frac{1}{2}}$.

We call this space *nr- Fock space* (non-relativistic Fock space) As measure spaces, the two Fock spaces *are not equivalent*.

In nr-Fock space the free hamiltonian is $\hat{H}_0 = \sum_n (-\Delta_n + m_n)^{\frac{1}{2}}$.

As usual we use the Krein as a way to explore the system.

In the non relativistic we introduce (weak) contact by a $::\phi^3(x)::$ interaction density as in Quantum Mechanics.

With the symbol $::.::$ we denote the normal ordered defined by the condition [L,S,T,T] that the last term (from the right) in the product is an annichilation operator and the first one is a creation operator (so that the choice is only in the middle term).

It a relativistically invariant definition. It has the consequence that the vacuum is invariant.

By construction the interaction hamiltonian has matrix elements only between states that contain at least one particle each.

Let $\psi_1(x)$ and $\psi_2(x)$ the wave functions of these two particles. Without loss of generality we choose $\psi_1 = \psi_2 \equiv \psi(x)$.

One is therefore back to contact of a particle with two identical particles.

We have discussed this case at length. Depending on the strength of the contact the system has a bound state or an Efimov sequence of bound states. .

We must now pass to the r-Fock space.

The topology of r-Foch space as measure space is weaker than that of nr-Fock space (the topology in r-Foch space is given by the relativistic hamiltonian, a first order differential operator, while the topology in a nr-Fock space is given by the non relativistic hamiltonian, a second order differential operator).

But also the covariance is different and the two effect concel.

Therefore, in r-Fock space there are bound states, states of fixed energy in any reference frame.

They correspond to particles.

frontiers in Physics

ORIGINAL RESEARCH
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Vacuum Energy for Generalized Dirac Combs at $T = 0$

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The quantum vacuum energy for a hybrid comb of Dirac δ-δ' potentials is computed by using the energy of the single δ-δ' potential over the real line that makes up the comb. The zeta function of a comb periodic potential is the continuous sum of zeta functions over the dual primitive cell of Bloch quasi-momenta. The result obtained for the quantum vacuum energy is non-perturbative in the sense that the energy function is not analytical for small couplings.

Keywords: quantum vacuum, casimir effect (theory), condensed matter, quantum field theories (QFT), selfadjoint extensions

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1. INTRODUCTION

In this paper we analyse a generalization of the Kronig-Penney model [1] in which the periodic point potential considered is a combination of the Dirac δ-potential and its first derivative, i.e., the δ-δ' potential (see ref. [2]). Note that the Kronig-Penney model is an example of a one dimensional exactly solvable periodic potential, widely used in Solid State Physics to describe electrons moving in an infinite periodic array of rectangular potential barriers. The δ-δ' potential has been a focus of attention over the last few years [3–7], but the δ-δ' comb as a classical background in interaction with a scalar quantum field has not been considered.

The main goal of this work is to compute the quantum vacuum energy of a scalar field propagating in a (1+1)-dimensional spacetime in interaction with the background of a generalized Dirac comb composed of δ-δ' potentials (see [2–4]). Interpreting the scalar field as electrons (disregarding spin) we would get a (non-additive) contribution to the internal energy of the lattice. In a periodic structure it is possible to calculate the quantum vacuum energy per unit cell, which gives a contribution to the internal pressure of the lattice. In addition, it is possible to interpret the quantum scalar field as phonons of the lattice. In such a case we would obtain the phonon contribution to the internal pressure of the lattice when computing the quantum vacuum energy per unit cell. However, since the (1+1)-dimensional quantum field theory is a highly simplified theoretical model we will not go into more detail about the interpretation.

Specifically, we study the one dimensional periodic Hamiltonian

$$\mathcal{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \qquad \text{where} \qquad V(x) = \sum_{n\in\mathbb{Z}} \mu\delta(x-nd) + 2\lambda\delta'(x-nd), \tag{1}$$

with couplings $\mu, \lambda \in \mathbb{R}$, and lattice spacing $d > 0$. We will work with dimensionless quantities defined as

$$y = \frac{mc}{\hbar}x, \qquad a = \frac{mc}{\hbar}d, \qquad w_0 = \frac{1}{\hbar c}\mu, \qquad w_1 = \frac{m}{\hbar^2}\lambda, \tag{2}$$

so that $[y, a, w_0, w_1] = 1$. In that way, the dimensionless time independent Schrödinger equation for the one-particle states of a quantum scalar field is

$$\left(-\frac{\partial^2}{\partial y^2}+V(y)\right)\phi(y)=k^2\phi(y),$$
$$V(y)=\sum_{n\in\mathbb{Z}} w_0\delta(y-na)+2w_1\delta'(y-na). \tag{3}$$

Its solutions enables us to determine the energy levels and energy bands of the crystal. Following ref. [8] the general form of the band equation in terms of scattering coefficients (t, r_R, r_L) for the compact supported potential from which the comb is built is

$$\cos(qa)=\frac{e^{iak}(t(k)^2-r_R(k)r_L(k))+e^{-iak}}{2t(k)}, \tag{4}$$

being q the quasi-momentum. This equation relates the quasi-momenta $q \in [-\pi/a, \pi/a]$ in the first Brillouin zone and the wave-vector k. The quasi-momentum determines the Bloch periodicity for a given wave function on the lattice:

$$\phi(y+a)=e^{iqa}\phi(y). \tag{5}$$

Since the cosine of the left hand side in (4) is a bounded function, the energy spectrum of the system is organized into allowed/forbidden energy bands/gaps. As a particular case, when the scattering data for a Dirac-δ potential $V = w_0\delta(x)$ on the line [9]

$$t_\delta(k)=\frac{2ik}{2ik-w_0},\quad r_\delta(k)=\frac{w_0}{2ik-w_0} \tag{6}$$

are plugged into equation (4) we obtain

$$\cos\big(qa\big)=\cos\big(ka\big)+\frac{w_0}{2k}\sin\big(ka\big) \tag{7}$$

which is the well known band equation for the Kronig-Penney model [1].

The general secular equation (4) will enable us to calculate the vacuum energy of the crystal. The vacuum energy per unit cell (in the interval $[0, a]$) is computed by spatially integrating the expectation value of the 00-component of the energy-momentum tensor $T_{\mu\nu}$:

$$E_0=\int_0^a dy\,\langle 0|\,T_{00}\,|0\rangle\,. \tag{8}$$

The non regularized infinite quantum vacuum energy can be represented as well as the summation over modes of the spectrum corresponding to the one-particle states of the field theory.

$$E_0=\int_0^a dy\,\langle 0|\,T_{00}\,|0\rangle=\sum_n k_n \tag{9}$$

being $\{\omega_n^2 = k_n\}$ the eigenvalues characterizing the one-particle states of the quantum field theory given by equation (4). The ultraviolet divergences that appear naturally in this expression must be subtracted taking into account the self-energy of the individual potential that makes up the comb and the fluctuations of the field in the chosen background. The calculation of $\langle 0|\,T_{00}\,|0\rangle$ provides the energy density per unit length within a unit cell. This of course contains much more information than just the total energy contained in a unit cell. Nevertheless, the calculation using Green functions will not be addressed in this paper for most general combs. On the other hand we can compute E_0 using spectral zeta functions [10] to skip the intermediate calculation of $\langle 0|\,T_{00}\,|0\rangle$ for which the exact Green function of the quantum field on the crystal is needed. When using the zeta function approach the infinite contributions are subtracted using the regularized expression for the quantum vacuum energy:

$$E_0(s)=\sum_n k_n^{-s}. \tag{10}$$

This expression is nothing but the spectral zeta function associated to the Schödinger operator defined in equation (3). In order to subtract the divergences one has to perform the analytic continuation of equation (10) for s to the whole complex plane, and then subtract the contribution of the pole at $s = -1$. A detailed explanation of how to proceed in most general cases is explained in refs. [10–12].

The structure of the present paper is the following. In section 2 we reproduce some basic results on spectral zeta functions that are needed throughout the paper. The section 3 provides a way to re-interpret a general comb formed by superposition of identical potentials with compact support centered at the lattice points, as a 1-parameter family of pistons mimicked by quasi-periodic boundary conditions using the formalism to characterise selfadjoint extensions developed in ref. [13]. Afterwards in section 4 and subsection 5.1, we will use the results from refs. [13, 14] to give a general formula for the finite quantum vacuum energy general comb formed by superposition of identical potentials with compact support. The subtraction of infinites follows from ref. [13]. The rest of section 5 is dedicated to the numerical results for the particular example of the δ-δ' comb, and the non-perturbative character inherent to the quantum vacuum energy of this particular example. Finally in section 6 we explain the conclusions of our paper.

2. SOME BASICS FORMULAS ON SPECTRAL ZETA FUNCTIONS

In general, given an arbitrary potential with *small*[1] support and its associated comb, the secular equation (4) can not be solved. Nevertheless, the summation over eigenvalues in (10) can be rewritten down using the residue theorem. In this section we explain the method to replace the summation over eigenvalues in equation (10) by a complex contour integral involving the logarithmic derivative of the function that defines the secular equation (4).

Let $\hat{H}$ be an elliptic non-negative selfadjoint, second order differential operator and $f_{\hat{H}}(z)$ an holomorphic function on $\mathbb{C}$

[1]Many of the results of this paper generalize straightforward to any comb built from a superposition of potentials with compact support centered at the lattice points, provided that the compact support of such potentials is smaller than the lattice spacing.

such that

i) $\lim_{z\to 0} f_{\hat{H}}(z) \neq 0, \infty$.

ii)If we define

$$Z(f_{\hat{H}}) \equiv \{k_n \in \mathbb{R}/f_{\hat{H}}(k_n) = 0\}$$
$$\tilde{\sigma}(\hat{H}) \equiv \{\lambda_n \in \mathbb{R}^+/\lambda_n \text{ is eigenvalue}\},$$

then $\forall k_n \in Z(f_{\hat{H}})$, $k_n^2 = \lambda_n \in \tilde{\sigma}(\hat{H})$. The multiplicity of k_n is the degeneracy of λ_n.

The formal definition of the spectral zeta function associated to $\hat{H}$ is

$$\zeta_{\hat{H}}(s) = \sum_{\tilde{\sigma}(\hat{H})} \lambda_n^{-s} \qquad \text{for Re(s)}> \text{ certain positive real number.} \tag{11}$$

Taking into account that the function

$$\frac{d}{dz}\log\big(f_{\hat{H}}(z)\big) \tag{12}$$

has poles at $Z(f_{\hat{H}})$ and that the residue coincides with the multiplicity of the corresponding zero, the summation over λ_n is equivalent to the summation over the zeroes of $f_{\hat{H}}(z)$ and therefore can be written as

$$\sum_{\tilde{\sigma}(\hat{H})}\{...\} = \sum_{Z(f_{\hat{H}})}\{...\} = \oint_C dz \frac{d}{dz}\log\big(f_{\hat{H}}(z)\big)\{...\} \tag{13}$$

where C is a contour that encloses all the zeroes contained in $Z(f_{\hat{H}})$. Since $\hat{H}$ is an elliptic non-negative selfadjoint, second order differential operator we can ensure $Z(f_{\hat{H}}) \subset \mathbb{R}$. Hence we can choose C to be the semicircle in the complex plane $[-iR, iR] \cup \{z \in \mathbb{C}/\ |z| = R,\ \text{and arg}(z) \in [-\pi, \pi]\}$ and then deform the contour taking the limit $R \to \infty$. After the limit is done, and with the properties assumed for $f_{\hat{H}}(z)$ we obtain an expression for the spectral zeta function that admits analytical continuation to the whole complex plane:

$$\zeta_{\hat{H}}(s) = \frac{\sin(\pi s)}{\pi}\int_0^\infty dk k^{-2s}\partial_k \log[f_{\hat{H}}(ik)]. \tag{14}$$

In this representation the information about the poles of $\zeta_{\hat{H}}(s)$ and the values at $s \in \mathbb{Z}$ is contained in

$$\frac{\sin(\pi s)}{\pi}\int_1^\infty dk k^{-2s}\partial_k \log[f_{\hat{H}}(ik)]. \tag{15}$$

Hence it all reduces to study (15) in order to obtain the pole structure (Res) and $\zeta_{\hat{H}}(s \in \mathbb{Z})$. In subsection 3.2 of ref. [14] it can be seen an example where all the calculations can be performed analytically.

3. THE COMB AS A PISTON

In order to perform the calculation of the quantum vacuum energy per unit cell for the comb, it is of great interest to re-interpret the corresponding quantum system as a one-parameter family of hamiltonians defined over the finite interval, by using general quantum boundary conditions in the formalism described in refs. [13, 15]. Bloch's theorem ensures that knowing the wave functions on a primitive cell is equivalent to the knowledge of the wave function in the whole lattice. Hence, if the origin of the real line is chosen in a way that it is coincident with one of the lattice potential centers, then it is enough to study the quantum mechanical system characterized by the quantum hamiltonian

$$H = -\frac{d^2}{dx^2} + w_0\delta(x) + 2w_1\delta'(x), \tag{16}$$

defined over the closed interval $[-a/2, a/2]$, being a the lattice spacing. Since the hamiltonian in (16) is not essentially selfadjoint when is defined over the square integrable functions over the closed interval $[-a/2, a/2]$ we need to impose boundary conditions at $x = \pm a/2$ over the boundary values $\{\psi(\pm a/2), \psi'(\pm a/2)\}$. If in addition such boundary condition ensures that the domain of the corresponding selfadjoint extension is a set of wave functions that satisfy Bloch's semi-periodicity condition[2], then we can understand the comb as a 1-parameter family of selfadjoint extensions where the parameter is to be interpreted as the quasi-momentum. Below we construct the family of selfadjoint extensions that model the comb.

To start with, let us study the δ-δ' potential sitting at $x = 0$ and confined in the interval [-a/2, a/2]. The hamiltonian of the system is given by (16) and its domain (the space of quantum states) in general would be characterized by the general boundary condition

$$\begin{pmatrix}\psi(-a/2) + i\psi'(-a/2)\\ \psi(a/2) - i\psi'(a/2)\end{pmatrix} = U\begin{pmatrix}\psi(-a/2) - i\psi'(-a/2)\\ \psi(a/2) + i\psi'(a/2)\end{pmatrix}, \tag{17}$$

where $U \in SU(2)$. In general any $U \in SU(2)$ makes (16) selfadjoint in the interval $[-a/2, a/2]$. Nevertheless, we are focused on mimicking with (17) Bloch's semi-periodicity condition:

$$\begin{aligned}\psi(a/2) &= e^{iqa}\psi(-a/2)\\ \psi'(a/2) &= e^{iqa}\psi'(-a/2).\end{aligned} \tag{18}$$

It is straightforward to see that the U that gives rise to (18) is given by

$$U_B = \begin{pmatrix}0 & e^{i\theta}\\ e^{-i\theta} & 0\end{pmatrix}. \tag{19}$$

Plugging (19) in (17) one gets

$$\begin{aligned}\psi(a/2) + i\psi'(a/2) &= e^{-i\theta}[\psi(-a/2) + i\psi'(-a/2)]\\ \psi(a/2) - i\psi'(a/2) &= e^{i\theta}[\psi(-a/2) - i\psi'(-a/2)].\end{aligned} \tag{20}$$

Adding and subtracting both expressions we obtain

$$\psi(a/2) = e^{-i\theta}\psi(-a/2)$$

[2]It is of note that in the interval $[-a/2, a/2]$, the subinterval $[-a/2, 0)$ belongs to one primitive cell, meanwhile the subinterval $(0, a/2]$ belongs to a different primitive cell.

$$\psi'(a/2) = e^{-i\theta}\psi'(-a/2), \tag{21}$$

and making $\theta = -qa$, we obtain the equations (18). Hence, the selfadjoint extension that gives Bloch's condition is given by

$$U_B = \begin{pmatrix} 0 & e^{-iqa} \\ e^{iqa} & 0 \end{pmatrix}. \tag{22}$$

In addition let us remember that the matching conditions that define the potential $V = w_0\delta(x) + 2w_1\delta'(x)$ are given by (see ref. [2])

$$\begin{pmatrix} \psi(0^+) \\ \psi'(0^+) \end{pmatrix} = \begin{pmatrix} \alpha & 0 \\ \beta & 1/\alpha \end{pmatrix} \begin{pmatrix} \psi(0^-) \\ \psi'(0^-) \end{pmatrix} \qquad \alpha = \frac{1+w_1}{1-w_1},$$
$$\beta = \frac{w_0}{1-w_1^2}. \tag{23}$$

When we solve the equation:

$$-\frac{d^2}{dx^2}\psi(x) = k^2\psi(x), \tag{24}$$

with the matching conditions (23) and the boundary condition (17) with $U = U_B$ given by (22) we can rearrange everything to write down the secular equation and the general solution in terms of the scattering data for the δ-δ' potential over the real line as was done in ref. [8]. This approach enables to interpret the δ-δ' comb as a one-parameter family of quantum pistons by reinterpreting the primitive cell of the comb in the following way:

1. The middle piston membrane is represented by the δ-δ' potential placed at $x = 0$. To ensure that the lattice quantum fields satisfy the matching conditions (23) we can assume the ansatz for the one-particle states wave functions in $[-a/2, a/2]$ is given by a linear combination of the two linear independent scattering states determined by the scattering amplitudes of the δ-δ' potential (see refs. [2–4])

$$t = \frac{-2k(w_1^2-1)}{2k(w_1^2+1)+iw_0}, \quad r_R = \frac{-4kw_1 - iw_0}{2k(w_1^2+1)+iw_0},$$
$$r_L = \frac{4kw_1 - iw_0}{2k(w_1^2+1)+iw_0}. \tag{25}$$

   From this amplitudes the determinant of the scattering matrix reads

$$\Rightarrow \det S_{\delta\delta'} = t^2 - r_R r_L = \frac{2k(w_1^2+1) - iw_0}{2k(w_1^2+1)+iw_0}. \tag{26}$$

2. The endpoints of the primitive cell correspond to the external walls of the piston placed at $x = \pm a/2$, and the quantum field satisfies the one-parameter family of quantum boundary conditions depending on the parameter $\theta = -qa$, which is the quasi-momentum, given by the unitary matrix U_B in (19).

The spectral function for $U = U_B$ written in terms of the scattering data (t, r_R, r_L) and the quasi-momentum q is (see formula 34 in ref. [8])

$$h(k) = 4k\,[2t\cos(qa) - e^{-ika} - e^{ika}(t^2 - r_R r_L)]. \tag{27}$$

The band structure of this comb is given by those k_j such that $h(k_j) = 0$. In general the solutions $\{k_0, k_1, ..., k_n, ...\}$ are functions of $q \in [-\pi/a, \pi/a]$, so $k_j(q)^2$ is an energy band when we let q take its continuum values in $[-\pi/a, \pi/a]$. In order to use zeta function regularization we need to remove in (27) the $4k$ global factor to get the "good" spectral function according to section 2 (see refs. [10, 14]). Hence the spectral function to be used in our zeta function regularization approach is given by

$$f_q(k) = 2t\left[\cos(qa) - \frac{1}{2t}(e^{-ika} + e^{ika}(t^2 - r_R r_L))\right]. \tag{28}$$

In (27) and (28), t, r_R, r_L are the scattering data for the compact supported potential from which the comb is built up on the real line. In addition it is trivial to see that

$$f_q(k) = 0 \quad \rightarrow \quad \cos(qa) = \frac{1}{2t}[e^{-ika} + e^{ika}(t^2 - r_R r_L)], \tag{29}$$

which is the usual form for the band equation written in standard text books such as [16], and generalized in [8]. Note that because $t^2 - r_R r_L$ is the determinant of the unitary scattering matrix, then $t(0)^2 - r_R(0)r_L(0) \neq 0$. Hence, in general we can work under the assumption that

$$\lim_{k\to 0} f_q(k) \neq 0, \infty. \tag{30}$$

REMARK

It is of note that all the formulas presented in this section, specially (28) is valid for any comb built from repetition of potentials with compact support smaller than the lattice spacing. All that is needed are the scattering amplitudes for a single potential of compact support over the real line, to obtain the corresponding spectral function that characterises the band structure of the corresponding comb.

4. SPECTRAL ZETA FUNCTION FOR THE CRYSTAL

Following the interpretation of the comb as a 1-parameter family of selfadjoint extensions given in the previous section we rethink the band spectrum in the following way

1. For a fixed value of $q \in [-\pi/a, \pi/a]$, $f_q(k) = 0$ with $f_q(k)$ given by (28), gives a discrete set of values of k in one-to-one correspondence with $\mathbb{N}$.
2. If we let q take values from $-\pi/a$ to π/a and put together all the discrete spectra from the previous item, then we will obtain all the allowed energy bands.

Hence in order to perform the calculation of the quantum vacuum energy for a massless scalar field we can write down the spectral zeta function that corresponds to the Schrödinger Hamiltonian of the comb

$$\sum_{bands} \int_{\sqrt{\epsilon^{(n)}_{min}}}^{\sqrt{\epsilon^{(n)}_{max}}} dk k^{-2s} = \int_{-\pi/a}^{\pi/a} \frac{dq\,a}{2\pi} \frac{\sin(\pi s)}{\pi} \int_0^\infty dk k^{-2s} \partial_k \log f_q(ik). \tag{31}$$

In this way we can write in general the spectral zeta function for the comb as

$$\zeta_C(s) = \frac{a}{2\pi}\int_{-\pi/a}^{\pi/a} dq \frac{\sin(\pi s)}{\pi}\int_0^\infty dk k^{-2s}\partial_k \log f_q(ik). \quad (32)$$

Since the integration in q runs over a finite interval, and q enters as a parameter of the selfadjoint extension associated to the unitary operator U_B in (22), all the infinite contributions of the quantum vacuum energy are enclosed in the zeta function for a δ-δ' potential placed at $x = 0$ confined between two plates placed at $x = \pm a/2$, i. e.

$$\zeta_q(s) = \frac{\sin(\pi s)}{\pi}\int_0^\infty dk k^{-2s}\partial_k \log f_q(ik). \quad (33)$$

As a result of the formulas for the spectral zeta function it is easy to conclude that the finite quantum vacuum energy for the comb, $E^{fin}_{\rm comb}$, can be obtained from the finite quantum vacuum energy $E^{fin}_0(q)$ for the quantum scalar field confined between two plates placed at $x = \pm a/2$ represented by the boundary condition associated to (22), and under the influence of a δ-δ' potential placed at $x = 0$:

$$E^{fin}_{\rm comb} = \frac{a}{2\pi}\int_{-\pi/a}^{\pi/a} dq E^{fin}_0(q). \quad (34)$$

Hence our problem reduces to compute $E^{fin}_0(q)$.

5. THE FINITE QUANTUM VACUUM ENERGY AT ZERO TEMPERATURE FOR GENERALIZED DIRAC COMBS

5.1. General Formulas

From this point we will use formula 2.26 in ref. [13] to obtain $E^{fin}_0(q)$. In ref. [13] there was no point potential between plates, so the final result arising there did not depend on the reference length L_0 used to subtract the infinite parts. In our case the existence of a potential with compact support between plates forces to take the limit $L_0 \to \infty$. Physically this limit means that what we subtract is the quantum vacuum energy of the potential with compact support on the whole real line. With these assumptions and changing the length L in ref. [13] by our lattice spacing a we can write

$$E^{fin}_0(q) = \lim_{a_0\to\infty}\frac{-a_0}{2\pi(a-a_0)}\times \int_0^\infty dk\, k\left[a - a_0 - \frac{d}{dk}\log\left(\frac{f^a_q(ik)}{f^{a_0}_q(ik)}\right)\right]. \quad (35)$$

In taking this limit, we must keep $qa = qa_0 = -\theta$ as a free parameter coming from the selfadjoint extension, and just after having done the limit and obtained a finite result make the replacement $\theta = -qa$. Hence to avoid confusion we can write

$$E^{fin}_0(\theta) = \lim_{a_0\to\infty}\frac{-a_0}{2\pi(a-a_0)}\int_0^\infty dk\, k\left[a - a_0 - \frac{d}{dk}\log\left(\frac{f^a_\theta(ik)}{f^{a_0}_\theta(ik)}\right)\right], \quad (36)$$

with

$$f^a_\theta(k) = 2t\left[\cos(\theta) - \frac{1}{2t}(e^{-ika} + e^{ika}(t^2 - r_R r_L))\right], \quad (37)$$

and finally

$$E^{fin}_{\rm comb} = \int_{-\pi}^{\pi}\frac{d\theta}{2\pi}E^{fin}_0(\theta), \quad (38)$$

being θ the parameter of the selfadjoint extension defined by U_B that is to be interpreted after obtaining a finite answer as $\theta = -qa$.

5.2. Some Comments on $E^{fin}_{\rm comb}$ and $E^{fin}_0(\theta)$

With the formulas written above for the finite quantum vacuum energy of the comb ($E^{fin}_{\rm comb}$) and the finite quantum vacuum interaction energy between two plates modeled by the boundary condition associated to U_B with a compact supported potential centered in the middle point of both plates ($E^{fin}_0(\theta)$), we are assuming that the zero point energy corresponds to the situation in which we have a free scalar quantum field over the real line. Under this assumption when the potential with compact support between plates is made identically zero ($t = 1, r_R = r_L = 0$), the quantity

$$\mathcal{E}_0(\theta) \equiv E^{fin}_0(\theta)\Big|_{t=1,r_R=r_L=0} \neq 0, \infty, \quad (39)$$

is nothing but the scalar quantum vacuum interaction energy between two plates mimicked by quasi-periodic boundary conditions. This was analytically obtained in refs. [13, 17] for the 1D, 2D, and 3D cases. The fact that $\mathcal{E}_0(\theta) \neq 0, \infty$ means that one would expect

$$E^{fin}_{\rm comb}(t = 1, r_R = r_L = 0) = \int_{-\pi}^{\pi}\frac{d\theta}{2\pi}\mathcal{E}_0(\theta) \neq 0, \infty, \quad (40)$$

which makes sense, since turning off the potential with compact support does not leave us with a quantum scalar field over the real line, because the Bloch periodicity condition remains. Nevertheless, if we take into account that any plane wave on the real line satisfies Bloch periodicity, the energy $E^{fin}_{\rm comb}(t = 1, r_R = r_L = 0)$ should be that of the free scalar field on the real line, i.e., zero. Knowing from refs. [17, 18] that

$$\mathcal{E}_0(\theta) = \frac{1}{2a}\left(|\theta| - \frac{\theta^2}{2\pi} - \frac{\pi}{3}\right),$$

it is straightforward to see that

$$E^{fin}_{\rm comb}(t = 1, r_R = r_L = 0) = \int_{-\pi}^{\pi}\frac{d\theta}{2\pi}\mathcal{E}_0(\theta) = 0. \quad (41)$$

As a result, we ensure that our general formula (38) gives total quantum vacuum energy for the comb identically zero when the potentials with compact support that form the comb are zero, as it should be.

5.3. E^{fin}_{comb} for the δ-δ' Comb

Plugging the scattering amplitudes given in (28) and after some algebraic manipulations we obtain

$$f_\theta(k) = -\frac{4k(1+w_1^2)}{\Delta_{\delta\delta'}}\left[\Omega\cos(\theta)+\cos(ka)+\frac{\gamma}{2k}\sin(ka)\right], \tag{42}$$

being $\Delta_{\delta\delta'} = [2k(w_1^2+1)+iw_0]^2$, $\Omega \equiv (w_1^2-1)/(w_1^2+1)$ and $\gamma \equiv w_0/(1+w_1^2)$. In order to have a well behaved spectral function ($f_\theta(k \to 0) \neq 0$) we have to remove the global $-4k(1+w_1^2)$ factor. In addition, the global factor $1/\Delta_{\delta\delta'}$ does not change the zeroes of the spectral function so it can also be dropped. Hence we obtain the following expression for the spectral function of the δ-δ' comb:

$$g_\theta(k) = \Omega\cos(\theta)+\cos(ka)+\frac{\gamma}{2k}\sin(ka). \tag{43}$$

The quantum vacuum energy is obtained from equation (38) after taking the limit $a_0 \to \infty$:

$$E^{fin}_{\delta\delta'\text{comb}} = \int_{-\pi}^{\pi}\frac{d\theta}{4\pi^2}\int_0^\infty dk\, F_{\delta\delta'}(k,\theta), \tag{44}$$

where

$$F_{\delta\delta'}(k,\theta) = \frac{A(k)}{B(k)+C(k)\cos\theta}+ak-\frac{\gamma}{\gamma+2k}, \tag{45}$$

and $A(k)$, $B(k)$, and $C(k)$ are defined as

$$A(k) = -ak\gamma\cosh(ka)+(-2ak^2+\gamma)\sinh(ka) \tag{46}$$

$$B(k) = 2k\cosh(ka)+\gamma\sinh(ka), \quad C(k) = 2k\Omega. \tag{47}$$

Since now everything is finite in (44) we can exchange the order of integration to do first the integration in θ

$$I_{\delta\delta'}(k) = \int_{-\pi}^{\pi}\frac{d\theta}{4\pi^2}F_{\delta\delta'}(k,\theta). \tag{48}$$

The integral in (48) can be obtained from ref. [19] (page 402 formula 3.645)

$$\int_0^\pi \frac{\cos^n(x)}{(b+\tau\cos x)^{n+1}} = \frac{\pi}{2^n(b+\tau)^n\sqrt{b^2-\tau^2}} \times\sum_{k=0}^{n}(-1)^k\frac{(2n-2k-1)!!(2k-1)!!}{(n-k)!k!}\left(\frac{\tau+b}{b-\tau}\right)^k,$$

for $b^2 > \tau^2$. In order to use this integral to obtain $I(k)$ in (48) we need to ensure that $B^2(k,a) > C^2(k,a)$. Taking into account the definition of $B(k), C(k)$ in (47), this condition is always fulfilled because $-1 < \Omega < 1$ and

$$\cosh(ka)+\frac{\gamma}{2k}\sinh(ka) > 1, \quad \forall k,a,\gamma > 0. \tag{49}$$

Hence the integration in θ is given by

$$I_{\delta\delta'}(k) = \frac{1}{2\pi}\left[\frac{A(k)}{\sqrt{B^2(k)-C^2(k)}}+ak-\frac{\gamma}{\gamma+2k}\right]. \tag{50}$$

With this result the quantum vacuum energy for the comb is finally reduced to a single integration in k :

$$E^{fin}_{\delta\delta'\text{comb}} = \int_0^\infty dk I_{\delta\delta'}(k). \tag{51}$$

This integral can be calculated numerically with *Mathematica*. The results are shown below. As can be seen in **Figure 2** the quantum vacuum energy produced by a quantum scalar field can be positive (repulsive force), negative (attractive force), or zero. Taking into account that the potentials sitting in each lattice node mimic atoms that have lost their most external electron, classically the force between them is repulsive (they all have positive charge). The fact that the quantum vacuum energy of the scalar field can be negative and hence reduce the repulsive classical force means that when the quantum vacuum energy is negative the lattice spacing tends to be smaller. On the other hand when the quantum vacuum force is positive the classical repulsion is enhanced promoting that the lattice spacing in the crystal becomes bigger. **Figure 1** shows the behavior of the quantum vacuum energy (51) as a function of the lattice spacing a. In all the cases shown the quantum vacuum energy becomes zero as $a \to \infty$ and tends to $\pm\infty$ as $a \to 0$. In addition it is very easy to check that in the limit $\gamma \to \infty$, i.e., $w_0 \to \infty$,

$$\lim_{\gamma\to\infty} I_{\delta\delta'}(k) = -\frac{ka\, e^{-ka}\,\text{csch}(ka)}{2\pi}, \tag{52}$$

one recovers the very well-known result for the quantum vacuum energy between two Dirichlet plates in $1+1$: $E_0 = -\pi/(24a)$. The limit $w_0 \to \infty$ gives the minimum quantum vacuum energy that the δ-δ' can have. On the other hand from **Figure 2** it is easy to see that the maximum energy is positive, and it occurs for $\Omega = \gamma = 0$, i.e., $w_1 = \pm 1$ and $w_0 = 0$. In this case

$$\lim_{\Omega,\gamma\to 0} I_{\delta\delta'}(k) = -\frac{ka(\tanh(ka)-1)}{2\pi} \Rightarrow$$
$$E^{fin}_{\delta\delta'\text{comb}}(\Omega=\gamma=0) = \frac{\pi}{48a}, \tag{53}$$

and it corresponds to mixed boundary conditions [20, 21], where Dirichlet boundary conditions are imposed on one side and Neumann ones on the other.

It is interesting to remark that, as it happens for the quantum vacuum interaction energy between two Dirac- δ plates in a $1+1$ dimensional scalar quantum field theory, the limit

$$\lim_{w_0\to 0} E^{fin}_{\delta\delta'\text{comb}}(\Omega=-1,w_0), \tag{54}$$

is not analytical in w_0 due to the infrared divergence that appears in the Feymann diagrams (see refs. [22, 23]). This can be seen in (50) if we take into account that the non analyticity is enclosed in the third term of the r.h.s.

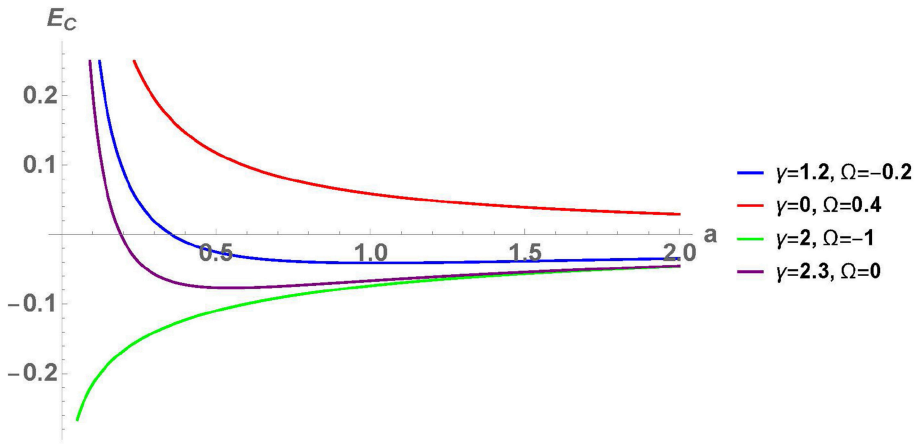

FIGURE 1 | Quantum vacuum energy as a function of the distance a for different values of the $\delta\delta'$ couplings.

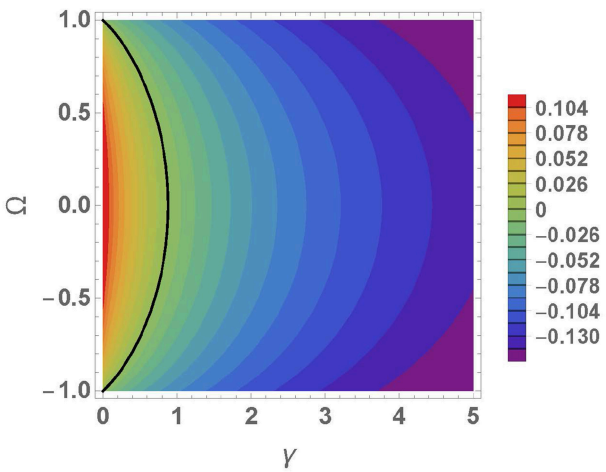

FIGURE 2 | Quantum vacuum energy for $a = 0.5$ in the coupling space γ-Ω. The black line represents the zero energy curve.

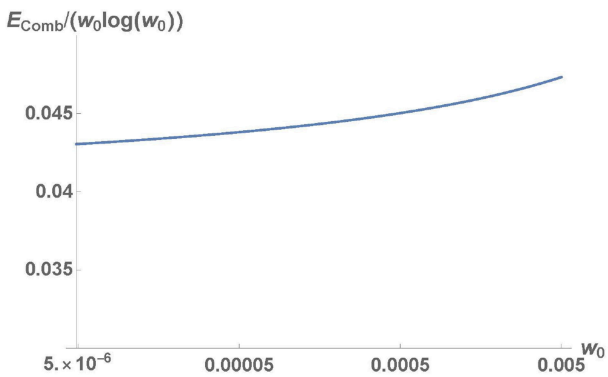

FIGURE 3 | Plot of $E^{fin}_{\delta\delta' comb}(\Omega = -1, w_0 \to 0)/(w_0 \log w_0)$ for $a = 1$. The w_0 axis is in logarithmic scale.

6. CONCLUSIONS AND FURTHER COMMENTS

We calculated the quantum vacuum energy of a comb formed by linear combinations of δ- and δ'-functions given in (1). The method presented in this paper is based on the spectral zeta function. We showed that the δ-δ' comb with lattice spacing a is equivalent to a single δ-δ' potential in the interval $[-a/2, a/2]$ at $x = 0$ together with a 1-parameter family of quasi-periodic boundary conditions at $x = \pm a/2$ given by (22). The band structure (27) arises when one takes into account that the spectrum of the comb is the set obtained by the union of all the discrete spectra of all the selfadjoint extensions obtained from the 1-parameter family of boundary conditions (22). The method can be easily generalized to any comb formed by the repetition of potentials with compact support, as long as the compact support is smaller than the lattice spacing. The ultraviolet divergences of these combs are the same as those of the quantum vacuum energy for one potential with compact support over the real line, which does not have a band structure but a continuum spectrum. Therefore, the ultraviolet divergences for the kind of combs studied in this paper do not depend on the lattice spacing. Subtracting these contributions we get a finite quantum vacuum energy that represents the part of the vacuum expectation value of the Hamiltonian of the quantum field theory, which depends on the lattice spacing. As expected, the generalized vacuum energy vanishes in the limit of infinite lattice spacing. This procedure has already been applied in ref. [24] for two δ-functions. The interpretation of this vacuum energy is a contribution (one-loop quantum correction) to the elastic lattice forces produced by the quantum scalar field of the phonons.

The calculations are to a large extent explicit. The result (51), has a fast converging single integration over k with the integrand (50), given in terms of elementary functions: exponential and hyperbolic functions. This integration is over imaginary frequency after performing a Wick rotation [24]. In addition, the result presented in (51) enables us to infer that when $w_1 = 0$,

i.e., $\Omega = -1$, the function $E^{fin}_{\delta\delta'\text{comb}}(\Omega = -1, \gamma = w_0)$ is not analytical when $w_0 \to 0$. Moreover, the plot in **Figure 3** shows that

$$E^{fin}_{\delta\delta'\text{comb}}(\Omega = -1, w_0 \to 0) \sim w_0 \log w_0, \tag{55}$$

as known from the vacuum energy of a single delta function (see refs. [22, 23]).

From this we can conclude that $E^{fin}_{\delta\delta'\text{comb}}(w_1, w_0)$ does not admit a perturbative expansion in powers of w_0 around $w_0 = 0$ when $w_1 = 0$. Hence the result given in formula (51) is non-perturbative in the sense that there is no power series expansion for $E^{fin}_{\delta\delta'\text{comb}}(\Omega = -1, w_0)$ when $w_0 \to 0$.

With a two-dimensional parameter space (the strength w_0 of the δ-potential and the strength w_1 of the δ'-potential) the quantum vacuum energy can be positive (repulsive force between nodes of the lattice) and negative (attractive force between nodes of the lattice). The interface between the two regimes mentioned is the line of zero quantum vacuum energy in the Ω-γ plane shown in **Figure 2**.

The techniques developed in this paper have provide a framework to calculate relevant quantities such as the free energy and the entropy at finite temperatures different from zero.

AUTHOR CONTRIBUTIONS

All authors listed have made a substantial, direct and intellectual contribution to the work, and approved it for publication.

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On the Spectra of One-Dimensional Schrödinger Operators With Singular Potentials

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The paper is devoted to the spectral properties of one-dimensional Schrödinger operators

$$S_q u(x) = \left(-\frac{d^2}{dx^2} + q(x)\right) u(x), \quad x \in \mathbb{R}, \tag{1}$$

with potentials $q = q_0 + q_s$, where $q_0 \in L^\infty(\mathbb{R})$ is a regular potential, and $q_s \in \mathcal{D}'(\mathbb{R})$ is a singular potential with support on a discrete infinite set $\mathcal{Y} \subset \mathbb{R}$. We consider the extension $\mathcal{H}$ of formal operator (1) to an unbounded operator in $L^2(\mathbb{R})$ defined by the Schrödinger operator S_{q_0} with regular potential q_0 and interaction conditions at the points of the set $\mathcal{Y}$. We study the closedness and self-adjointness of $\mathcal{H}$. If the set $\mathcal{Y} \simeq \mathbb{Z}$ has a periodic structure we give the description of the essential spectrum of operator $\mathcal{H}$ in terms of limit operators. For periodic potentials q_0 we consider the Floquet theory of $\mathcal{H}$, and apply the spectral parameter power series method for determining the band-gap structure of the spectrum. We also consider the case when the regular periodic part of the potential is perturbed by a slowly oscillating at infinity term. We show that this perturbation changes the structure of the spectra of periodic operators significantly. This works presents several numerical examples to demonstrate the effectiveness of our approach.

Keywords: periodic Schrödinger operators, limit operators method, spectral parameter power series (SPPS) method, dispersion equation, monodromy matrices, slowly oscillating at infinity perturbation

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1. INTRODUCTION

We consider formal one-dimensional Schrödinger operators

$$S_q u(x) = \left(-\frac{d^2}{dx^2} + q(x)\right) u(x), \quad x \in \mathbb{R} \tag{2}$$

with potentials $q = q_0 + q_s$, where $q_0 \in L^\infty(\mathbb{R})$ is a regular potential and $q_s \in \mathcal{D}'(\mathbb{R})$ is a singular potential with support on an infinite discrete set $\mathcal{Y} \subset \mathbb{R}$. The Schrödinger operator S_q is a far-reaching generalization of the well-known Kronig-Penney Hamiltonian

$$\mathcal{H} = -\frac{d^2}{dx^2} + \sum_{\gamma \in \mathbb{Z}} \alpha \delta(x - \gamma), \quad \alpha \in \mathbb{R}$$

describing the electron propagation in one-dimensional crystals [1, 2]. There exists an extensive literature devoted to the different spectral problems of one-dimensional Schrödinger operators with singular potentials (see, e.g., [3–9]).

Let $\mathcal{Y} = \{y_j\}_{j\in\mathbb{Z}}$ be a sequence of points $y_j \in \mathbb{R}$ such that $y_j < y_{j+1}$ for every $j \in \mathbb{Z}$, $e_j = (y_j, y_{j+1})$, $j \in \mathbb{Z}$, and $|e_j| = y_{j+1} - y_j$, $j \in \mathbb{Z}$, is the length of e_j. We assume that

$$0 < \inf_{j\in\mathbb{Z}} |e_j| \le \sup_{j\in\mathbb{Z}} |e_j| < \infty.$$

Let the formal Schrödinger operator (2) have the potential $q = q_0 + q_s$, where $q_0 \in L^\infty(\mathbb{R})$ and

$$q_s(x) = \sum_{y\in\mathcal{Y}} \left(\alpha(y)\,\delta(x-y) + \beta(y)\,\delta'(x-y)\right) \tag{3}$$

is a singular potential, which is a distribution in $\mathcal{D}'(\mathbb{R})$ with support at $\mathcal{Y}$. We assume that the functions $\alpha(y)$, $\beta(y)$ belong to the space $l^\infty(\mathcal{Y})$ with the norm $\|u\|_{l^\infty(\mathcal{Y})} = \sup_{y\in\mathcal{Y}} |u(y)|$.

Note that the operator S_q coincides with the operator S_{q_0} on the space $C_0^\infty(\mathbb{R}\setminus\mathcal{Y})$. Following the Kurasov paper [9] we consider the extension of $S_q|_{C_0^\infty(\mathbb{R}\setminus\mathcal{Y})}$ to the unbounded operator $\mathcal{H}_{q_0}$ in $L^2(\mathbb{R})$ defined by the Schrödinger operator S_{q_0} with domain $\mathrm{Dom}\mathcal{H}_{q_0} = \widetilde{H}^2(\Gamma)$, being

$$\widetilde{H}^2(\Gamma) = \left\{u \in H^2(\Gamma) : \begin{pmatrix} u(y^+) \\ u'(y^+)\end{pmatrix} = \mathbf{A}(y)\begin{pmatrix} u(y^-) \\ u'(y^-)\end{pmatrix},\ \forall y \in \mathcal{Y}\right\},$$

where $\Gamma = \mathbb{R}\setminus\mathcal{Y} = \bigcup_{j\in\mathbb{Z}} e_j$, $H^2(\Gamma) = \bigoplus_{j\in\mathbb{Z}} H^2(e_j)$, being $H^2(e_j)$ the Sobolev spaces of the order 2 on the intervals e_j, $u(y^\pm) = \lim_{\varepsilon\to+0} u(y\pm\varepsilon)$, $u'(y^\pm) = \lim_{\varepsilon\to+0} u'(y\pm\varepsilon)$, and

$$\mathbf{A}(y) = \begin{pmatrix} a_{11}(y) & a_{12}(y) \\ a_{21}(y) & a_{22}(y)\end{pmatrix}$$

is a complex 2×2-matrix with entries $a_{ij}(y) \in l^\infty(\mathcal{Y})$, $i,j = 1,2$. For potential (3) the matrix $\mathbf{A}(y)$ is of the form

$$\mathbf{A}(y) = \begin{pmatrix} \frac{4-\alpha(y)\beta(y)}{4+\alpha(y)\beta(y)} & \frac{-4\beta(y)}{4+\alpha(y)\beta(y)} \\ \frac{4\alpha(y)}{4+\alpha(y)\beta(y)} & \frac{4-\alpha(y)\beta(y)}{4+\alpha(y)\beta(y)}\end{pmatrix},\ \alpha(y)\beta(y) \ne -4,\quad y\in\mathcal{Y}.$$

The following results are obtained in the paper:

1. We prove an *a priori* estimate for the operator S_{q_0} of the form

$$\|u\|_{\widetilde{H}^2(\Gamma)} \le C\left(\|S_{q_0}u\|_{L^2(\mathbb{R})} + \|u\|_{L^2(\mathbb{R})}\right),\quad u\in\widetilde{H}^2(\Gamma).$$

   This estimate implies that the operator $\mathcal{H}_{q_0}$ is closed. Moreover, if the potential q_0 and the entries of the matrix $\mathbf{A}(y)$ are real-valued such that $\det\mathbf{A}(y) = 1$ for every $y \in \mathcal{Y}$, the operator $\mathcal{H}_{q_0}$ is self-adjoint.
2. Let the set $\mathcal{Y}$ of the singular points of the potential q to have a periodic structure. This means that the set $\mathcal{Y}$ is invariant with respect to the group $\mathbb{G} = \ell\mathbb{Z}$, $\ell > 0$. Let $\{g_m\}$ be a sequence of points of the group $\mathbb{G}$ tending to ∞. We associate with $\{g_m\}$ the operator-valued sequence $\{V_{-g_m}\mathcal{H}_{q_0}V_{g_m}\}$. We define the limit operators $\mathcal{H}_{q^g}$, which are the limits in some sense of the operator sequences $\{V_{-g_m}\mathcal{H}_{q_0}V_{g_m}\}$, where $V_h u(x) = u(x-h)$, $x\in\mathbb{R}$, $h\in\mathbb{G}$ is the shift operator. Then we give the general description of the essential spectrum $\mathrm{sp}_{\mathrm{ess}}\mathcal{H}_{q_0}$ in terms of the limit operators.
3. Let every sequence $\mathbb{G}\ni g_m\to\infty$ have a subsequence $\mathbb{G}\ni h_m\to\infty$ defining a limit operator $\mathcal{H}_{q_0^h}$. Then we prove that

$$\mathrm{sp}_{\mathrm{ess}}\mathcal{H}_{q_0} = \bigcup_{\mathcal{H}_{q_0^h}\in\mathrm{Lim}(\mathcal{H}_{q_0})} \mathrm{sp}\mathcal{H}_{q_0^h}, \tag{4}$$

   where $\mathrm{Lim}(\mathcal{H}_{q_0})$ is the set of all limit operators of $\mathcal{H}_{q_0}$.
4. Periodic structures. Let the potential $q_0(x)$, $x\in\mathbb{R}$, and the matrix $\mathbf{A}(y)$, $y\in\mathcal{Y}$, be periodic with respect to the group $\mathbb{G}$ and real-valued. Moreover, we assume that $\det\mathbf{A}(y) = 1$ for all $y\in\mathcal{Y}$. Then $\mathcal{H}_{q_0}$ is a self-adjoint operator and formula (4) yields

$$\mathrm{sp}_{\mathrm{ess}}\mathcal{H}_{q_0} = \mathrm{sp}\mathcal{H}_{q_0}.$$

   On applying the Floquet transform we obtain that

$$\mathrm{sp}\mathcal{H}_{q_0} = \{\lambda\in\mathbb{R} : |D(\lambda)| \le 1\},$$

   where $D(\lambda) = \frac{1}{2}\left(\varphi_1(\ell,\lambda) + (\varphi_2)'_x(\ell,\lambda)\right)$ is a function defined from a pair of linearly independent solutions φ_1, φ_2 of the Schrödinger equation $S_{q_0}u(x) = \lambda u(x)$, $x\in[0,\ell)$, which satisfy the Cauchy conditions $\varphi_1(0,\lambda) = 1$, $(\varphi_1)'_x(0,\lambda) = 0$, $\varphi_2(0,\lambda) = 0$, $(\varphi_2)'_x(0,\lambda) = 1$, as well as interaction conditions at the points $y\in\mathcal{Y}_0\subset[0,\ell)$. In the paper we obtain an explicit expression for function D in terms of monodromy matrices associated to the point interactions from the singular potential (3). Entries of monodromy matrices are calculated by means of the SPPS method [10], which allows to consider arbitrary regular potentials q_0 satisfying certain smoothness conditions. This approach in turn leads to an effective numerical method for calculating the edges of the spectral bands of Schrödinger operators $\mathcal{H}_{q_0}$.
5. Slowly oscillating at infinity perturbations of periodic potentials. We say that a function $a\in L^\infty(\mathbb{R})$ is slowly oscillating at infinity and belongs to the class $\mathrm{SO}(\mathbb{R})$ if

$$\lim_{x\to\infty}\sup_{x'\in K}|a(x+x') - a(x)| = 0$$

   for every compact set $K\subset\mathbb{R}$. As above we assume that the set $\mathcal{Y}$ is invariant with respect to the group $\mathbb{G}$. We apply formula (4) for the investigation of the perturbation of the periodic operators $\mathcal{H}_q$ by adding to the potential $q_0\in L^\infty(\mathbb{R})$ a slowly oscillating term $q_1\in\mathrm{SO}(\mathbb{R})$. Let $\mathcal{H}_{q_0}$ be a periodic operator with respect to the group $\mathbb{G}$ given by the Schrödinger operator S_{q_0} with $\mathbb{G}$-periodic real-valued potential q_0 and the $\mathbb{G}$-periodic real matrices $\mathbf{A}(y)$ satisfying $\det\mathbf{A}(y) = 1$ for every $y\in\mathcal{Y}$. We consider the operator $\mathcal{H}_{q_0+q_1}$, where

$q_1 \in \mathrm{SO}(\mathbb{R})$ is a real-valued function. Note that the operator $\mathcal{H}_{q_0}$ has a band-gap spectrum

$$\mathrm{sp}\mathcal{H}_{q_0} = \bigcup_{k=1}^{\infty} [a_k, b_k], \quad b_k \leq a_{k+1},\ k \in \mathbb{N}.$$

The limit operators of the operator $\mathcal{H}_{q_0+q_1}$ are of the form $\mathcal{H}^h_{q_0+q_1} = \mathcal{H}_{q_0+q_1^h}$, where $q_1^h \in \mathbb{R}$. Hence

$$\mathrm{sp}\mathcal{H}_{q_0+q_1^h} = \bigcup_{k=1}^{\infty} \left[a_k + q_1^h, b_k + q_1^h\right].$$

Applying formula (4) we obtain the essential spectrum of the operator $\mathcal{H}_{q_0+q_1}$ as

$$\mathrm{sp}_{\mathrm{ess}}\mathcal{H}_{q_0+q_1} = \bigcup_{k=1}^{\infty} [a_k + m_{q_1}, b_k + M_{q_1}],$$

where $m_{q_1} = \liminf_{x\to\infty} q_1(x)$, $M_{q_1} = \limsup_{x\to\infty} q_1(x)$. Above formula shows that if the oscillation of q_1 at infinity is large enough, that is $a_{k+1} - b_k < M_{q_1} - m_{q_1}$, the gap (b_k, a_{k+1}) of the spectrum of periodic operator $\mathcal{H}_{q_0}$ disappears in $\mathrm{sp}_{\mathrm{ess}}\mathcal{H}_{q_0+q_1}$. Hence, the slowly oscillating perturbations of the periodic potentials can substantially change the structure of the essential spectrum of $\mathcal{H}_{q_0}$.

6. Numerical calculation of the spectra of Schrödinger operator with periodic point interactions. We consider several examples for showing the application of the theory here presented, and calculate approximations of their corresponding spectra.

Notations

We will use the standard notations: $C^\infty(\mathbb{R})$ is the space of infinitely differentiable functions on $\mathbb{R}$, $C_b^\infty(\mathbb{R})$ is a subspace of $C^\infty(\mathbb{R})$ of functions with all bounded derivatives on $\mathbb{R}$, $\mathcal{D}(\mathbb{R}) = C_0^\infty(\mathbb{R})$ is a subspace of $C^\infty(\mathbb{R})$ consisting of functions with compact support, $\mathcal{D}'(\mathbb{R})$ is the space of distributions under $\mathcal{D}(\mathbb{R})$. We denote by $H^s(\mathbb{R})$, $s \in \mathbb{R}$, the Sobolev space with the norm

$$\|u\|_{H^s(\mathbb{R})} = \left(\int_{\mathbb{R}} \left(1+\xi^2\right)^s \left|\hat{u}(\xi)\right|^2 \mathrm{d}\xi\right)^{1/2},$$

where $\hat{u}(\xi)$ is the Fourier transform of $u(x)$. If $\Omega \subseteq \mathbb{R}$ is an open set, then $H^s(\Omega)$ is the space of restrictions on Ω of functions on $\mathbb{R}$ with the standard norm of restriction.

If exist, we denote the one-sided limits of f at x_0 by

$$f\left(x_0^-\right) := \lim_{\substack{x\to x_0,\\ x<x_0}} f(x), \qquad f\left(x_0^+\right) := \lim_{\substack{x\to x_0,\\ x>x_0}} f(x),$$

and by $\left[f\right]_{x_0} := f\left(x_0^+\right) - f\left(x_0^-\right)$ the (finite) jump of f at x_0.

Let X, Y be Banach spaces, then $\mathcal{B}(X,Y)$ is the space of all bounded linear operators acting from X into Y, and $\mathcal{K}(X,Y)$ is a subspace of $\mathcal{B}(X,Y)$ consisting of all compact operators acting from X into Y. If $X = Y$ we simply write $\mathcal{B}(X)$ and $\mathcal{K}(X)$, respectively.

Let A be an unbounded closed operator in a Hilbert space H with domain $\mathrm{Dom}(A)$ dense in H. The essential spectrum $\mathrm{sp}_{\mathrm{ess}}A$ of operator A is the set of numbers $\lambda \in \mathbb{C}$ for which the operator $A - \lambda$ is not Fredholm as an unbounded operator in H. If A is self-adjoint in H then its discrete spectrum is given by $\mathrm{sp}_{\mathrm{dis}}A = \mathrm{sp}A \setminus \mathrm{sp}_{\mathrm{ess}}A$, where $\mathrm{sp}A$ denotes the spectrum of A.

2. ONE-DIMENSIONAL SCHRÖDINGER OPERATORS WITH POINT INTERACTIONS

In this section we consider one-dimensional Schrödinger operators with potentials involving a countable set of point interactions and investigate some of their functional properties such as closedness, self-adjointness, Fredholmness, as well as their essential spectrum.

2.1. A Self-Adjoint Extension of Schrödinger Operators With a Point Interaction

Let us consider a singular distribution

$$q_s(x) = \alpha\delta(x) + \beta\delta'(x), \tag{5}$$

which represents a point interaction with support at $x = 0$. By the definitions

$$\delta(x)\,u(x) = \delta(u)\,\delta(x) = u(0)\,\delta(x),$$

and

$$\delta'(x)\,u(x) = \delta'(u)\,\delta'(x) = -u'(0)\,\delta'(x),$$

it follows that the action of q_s on the test functions in $\mathcal{D}(\mathbb{R})$ is defined by

$$q_s u = \alpha u(0)\,\delta(x) - \beta u'(0)\,\delta'(x).$$

In the study of Schrödinger operators involving point interactions we define a space of discontinuous test functions at $x = 0$,

$$D_0(\mathbb{R}) := C_0^\infty\left(\overline{\mathbb{R}_+}\right) \oplus C_0^\infty\left(\overline{\mathbb{R}_-}\right)$$

where $\mathbb{R}_\pm := \{x \in \mathbb{R} : x \gtrless 0\}$, and $C_0^\infty\left(\overline{\mathbb{R}_\pm}\right)$ are the spaces of restrictions on $\overline{\mathbb{R}_\pm}$ of functions in $C_0^\infty(\mathbb{R})$. Continuations of δ- and δ'-distributions on functions in $D_0(\mathbb{R})$ are defined as follows

$$\widetilde{\delta}(u) := \frac{u\left(0^+\right) + u\left(0^-\right)}{2}, \quad \widetilde{\delta}'(u) := -\frac{u'\left(0^+\right) + u'\left(0^-\right)}{2}, \quad u \in D_0(\mathbb{R}).$$

If $u \in \mathcal{D}(\mathbb{R})$ it follows that $\widetilde{\delta}(u) = \delta(u)$ and $\widetilde{\delta}'(u) = \delta'(u)$.

Let us consider the formal one-dimensional Schrödinger operator

$$S_q u(x) = \left(-\frac{d^2}{dx^2} + q(x)\right) u(x), \qquad x \in \mathbb{R}, \tag{6}$$

where $q = q_s + q_0$, with $q_0 \in L^\infty(\mathbb{R})$ as a regular potential, and $q_s \in \mathcal{D}'(\mathbb{R})$ as a singular potential defined in (5). Note that operator S_q coincides with operator S_{q_0} on the space $C_0^\infty(\mathbb{R}\setminus\{0\})$. A domain $\mathrm{Dom}(S_q)$ of operator S_q as an unbounded operator in $L^2(\mathbb{R})$ must consist of functions $u \in L^2(\mathbb{R})$ such that $S_q u \in L^2(\mathbb{R})$. This condition is fulfilled by functions $u \in D_0(\mathbb{R})$ satisfying at the origin the following interaction conditions

$$\begin{pmatrix} u(0^+) \\ u'(0^+) \end{pmatrix} = \mathbf{A}_0 \begin{pmatrix} u(0^-) \\ u'(0^-) \end{pmatrix}, \quad \mathbf{A}_0 = \begin{pmatrix} \frac{4-\alpha\beta}{4+\alpha\beta} & \frac{-4\beta}{4+\alpha\beta} \\ \frac{4\alpha}{4+\alpha\beta} & \frac{4-\alpha\beta}{4+\alpha\beta} \end{pmatrix}, \ \alpha\beta \neq -4,$$

where matrix $\mathbf{A}_0$ satisfies $\det \mathbf{A}_0 = 1$.

The embedding theorem for Sobolev space implies that if $u \in H^2(\mathbb{R}\setminus\{0\}) := H^2(\mathbb{R}_+) \oplus H^2(\mathbb{R}_-)$ the one-sided limits $u(0^\pm)$, $u'(0^\pm)$ exist, and the jumps $[u]_0$, $[u']_0$ are well defined. Let $\mathcal{H}_{q_0}$ be the unbounded operator in $L^2(\mathbb{R})$ defined by the Schrödinger operator $S_{q_0} = -\frac{d^2}{dx^2} + q_0$ with domain $\mathrm{Dom}(\mathcal{H}_{q_0}) = \widetilde{H}^2(\mathbb{R}\setminus\{0\})$ where

$$\widetilde{H}^2(\mathbb{R}\setminus\{0\}) = \left\{ u \in H^2(\mathbb{R}\setminus\{0\}) : \begin{pmatrix} u(0^+) \\ u'(0^+) \end{pmatrix} = \mathbf{A}_0 \begin{pmatrix} u(0^-) \\ u'(0^-) \end{pmatrix} \right\}.$$

If $q_0 \in L^\infty(\mathbb{R})$ is a real-valued function, $\mathbf{A}_0$ is a real 2×2-matrix, and $\det \mathbf{A}_0 = 1$, then $\mathcal{H}_{q_0}$ is a self-adjoint operator. We will prove this result in a more general setting in forthcoming Theorem 2. Thus the unbounded operator $\mathcal{H}_{q_0}$ generated by the Schrödinger operator S_{q_0} with domain $\widetilde{H}^2(\mathbb{R}\setminus\{0\})$ is a self-adjoint extension of formal Schrödinger operator $S_{q_0+q_s}$.

Schrödinger operators involving point interactions of the form $q_s(x) = \alpha\delta(x) + \beta\delta'(x)$ have been considered as norm resolvent approximations of certain families of Schrödinger operators with potentials depending on parameters tending to zero. The norm resolvent convergence of such families of operators was established and a class of solvable models that approximate the quantum systems was obtained in the works [11–13].

2.2. Properties of Schrödinger Operators With a Countable Set of Point Interactions

Let $\mathcal{Y} = \{y_j\}_{j\in\mathbb{Z}}$ be a sequence of real numbers such that $y_j < y_{j+1}$ for every $j \in \mathbb{Z}$. We denote by $e_j := (y_j, y_{j+1})$, $j \in \mathbb{Z}$, the corresponding interval between a pair of adjacent points y_j and y_{j+1}. The interval e_j has a length $|e_j| := y_{j+1} - y_j$, such that

$$0 < \inf_{j\in\mathbb{Z}} |e_j| \le \sup_{j\in\mathbb{Z}} |e_j| < \infty.$$

We denote

$$\Gamma := \mathbb{R}\setminus\mathcal{Y} = \bigcup_{j\in\mathbb{Z}} e_j, \quad \text{and} \quad H^2(\Gamma) := \bigoplus_{j\in\mathbb{Z}} H^2(e_j).$$

Let us consider the Schrödinger operator S_q defined in (6) with the regular potential $q_0 \in L^\infty(\mathbb{R})$, and the singular potential

$$q_s(x) = \sum_{y\in\mathcal{Y}} \left(\alpha(y)\,\delta(x-y) + \beta(y)\,\delta'(x-y)\right), \qquad (7)$$

which is a distribution in $\mathcal{D}'(\mathbb{R})$ with support at $\mathcal{Y} \subset \mathbb{R}$. We assume that $\alpha, \beta \in l^\infty(\mathcal{Y})$, where the space $l^\infty(\mathcal{Y})$ consists of all bounded complex-valued functions on the set $\mathcal{Y}$, which is equipped by the norm $\|u\|_{l^\infty(\mathcal{Y})} := \sup_{y\in\mathcal{Y}} |u(y)|$. Note that the operator S_q coincides with the Schrödinger operator $S_{q_0} := -\frac{d^2}{dx^2} + q_0$ on the space $C_0^\infty(\Gamma) := \bigoplus_{j\in\mathbb{Z}} C_0^\infty(e_j)$. Following the ideas of the work [9], the operator S_q defined on $C_0^\infty(\Gamma)$ is extended to an unbounded operator $\mathcal{H}_{q_0}$ in $L^2(\mathbb{R})$ defined by the Schrödinger operator S_{q_0} with domain $\mathrm{Dom}(\mathcal{H}_{q_0}) = \widetilde{H}^2(\Gamma)$, where $\widetilde{H}^2(\Gamma)$ is a subspace of $H^2(\Gamma)$ given by

$$\widetilde{H}^2(\Gamma) = \left\{ u \in H^2(\Gamma) : \quad \begin{pmatrix} u(y^+) \\ u'(y^+) \end{pmatrix} = \mathbf{A}(y) \begin{pmatrix} u(y^-) \\ u'(y^-) \end{pmatrix}, \quad \forall\, y \in \mathcal{Y} \right\},$$

where

$$\mathbf{A}(y) = \begin{pmatrix} a_{11}(y) & a_{12}(y) \\ a_{21}(y) & a_{22}(y) \end{pmatrix}, \quad y \in \mathcal{Y},$$

are complex 2×2-matrices with entries $a_{ij} \in l^\infty(\mathcal{Y})$ $(i,j = 1,2)$. In the case of potential (7), the corresponding matrices are of the form

$$\mathbf{A}(y) := \begin{pmatrix} \frac{4-\alpha(y)\beta(y)}{4+\alpha(y)\beta(y)} & \frac{-4\beta(y)}{4+\alpha(y)\beta(y)} \\ \frac{4\alpha(y)}{4+\alpha(y)\beta(y)} & \frac{4-\alpha(y)\beta(y)}{4+\alpha(y)\beta(y)} \end{pmatrix}, \qquad \alpha(y)\,\beta(y) \neq -4,\ y \in \mathcal{Y},$$

which satisfy $\det \mathbf{A}(y) = 1$, for every $y \in \mathcal{Y}$.

If the conditions:

1. regular potential $q_0 \in L^\infty(\mathbb{R})$, and
2. matrices $\mathbf{A}(y) = (a_{ij}(y))_{i,j=1}^2$ are such that $a_{ij} \in l^\infty(\mathcal{Y})$ for every $y \in \mathcal{Y}$

are fulfilled, then the operator S_{q_0} is bounded from $\widetilde{H}^2(\Gamma)$ into $L^2(\mathbb{R})$. Let us consider the following results for Schrödinger operators involving a countable set of point interactions.

Theorem 1 (An *a priori* estimate)**.** *Let* $\inf_{j\in\mathbb{Z}} |e_j| > 0$*, and conditions (1), (2) be satisfied. Then, there exists a constant* $C > 0$ *such that for every function* $u \in \widetilde{H}^2(\Gamma)$ *the following estimate*

$$\|u\|_{\widetilde{H}^2(\Gamma)} \le C\left(\|S_{q_0}u\|_{L^2(\mathbb{R})} + \|u\|_{L^2(\mathbb{R})}\right) \qquad (8)$$

holds.

Proof: *A priori* estimate (8) is proved similarly as in the theory of general boundary-value problems (see, e.g., [14]), but instead of a finite partition of unity we use a countable partition of unity of finite multiplicity. The proof is similar to that of Theorem 3.1 in Rabinovich [15].

Theorem 1 implies the following propositions.

Proposition 1 (Closedness)**.** *Let conditions (1), (2) hold. Then, the operator* $\mathcal{H}_{q_0}$ *is closed in* $L^2(\mathbb{R})$.

Proposition 2 (Parameter dependent Schrödinger operators)**.** *Let*

$$S_{\mu^2}u(x) := -\frac{d^2u(x)}{dx^2} + \mu^2 u(x), \quad x \in \Gamma,\ \mu > 0$$

be a Schrödinger operator acting from $\widetilde{H}^2(\Gamma)$ *into* $L^2(\mathbb{R})$. *We assume that the entries of matrices* $\mathbf{A}(y)$, $y \in \mathcal{Y}$, *are real-valued, and* $\liminf_{y\to\infty} |a_{12}(y)| > 0$ *or there exists a finite set* $\mathcal{N} \subset \mathcal{Y}$ *such that* $a_{12}(y) = 0$ *for every* $y \in \mathcal{Y} \setminus \mathcal{N}$. *Then, there exists* $\mu_0 > 0$ *such that the operator* $S_{\mu^2} : \widetilde{H}^2(\Gamma) \to L^2(\mathbb{R})$ *is invertible for every* $\mu \geq \mu_0$.

Proof: To prove this proposition we follow the approach of the well-known paper [16] where the authors studied general elliptic boundary-value problems depending on a parameter in bounded domains in $\mathbb{R}^n$. Similarly to the proof of Theorem 1, here we use a partition of unity and construct local inverses depending on a parameter, and then we form the global inverse operator by *sticking* these inverses for large values of the parameter. Unlike the paper [16], here we use a countable partition of unity of finite multiplicity, and follow the proof of Proposition 2 in Rabinovich [17].

Theorem 2 (Self-adjointness). *Let* $q_0 \in L^\infty(\mathbb{R})$ *be real-valued, and let matrices* $\mathbf{A}(y) = \left(a_{ij}(y)\right)_{i,j=1}^2$ *possess real-valued entries* $a_{ij} \in l^\infty(\mathcal{Y})$. *We assume: (i)* $\liminf_{y\to\infty} |a_{12}(y)| > 0$ *or there exists a finite set* $\mathcal{N} \subset \mathcal{Y}$ *such that* $a_{12}(y) = 0$ *for every* $y \in \mathcal{Y} \setminus \mathcal{N}$; *(ii)* $\det \mathbf{A}(y) = 1$, *for every* $y \in \mathcal{Y}$. *Then, the unbounded operator* $\mathcal{H}_{q_0}$ *defined by the Schrödinger operator* $S_{q_0} = -\frac{d^2}{dx^2} + q_0$ *with domain* $\widetilde{H}^2(\Gamma)$ *is self-adjoint in* $L^2(\mathbb{R})$.

Proof: Let $u, v \in \mathrm{Dom}(\mathcal{H}_q)$. On applying integration by parts twice we obtain

$$\int_\Gamma S_q u(x)\,\overline{v}(x)\,dx = \int_\Gamma u(x)\,S_q\overline{v}(x)\,dx + \sum_{y\in\mathcal{Y}} \left(\left[u\overline{v'}\right]_y - \left[u'\overline{v}\right]_y \right).$$

Note that

$$\begin{aligned}\left[u\overline{v'}\right]_y - \left[u'\overline{v}\right]_y &= \left(u(y^+)\,\overline{v'}(y^+) - u(y^-)\,\overline{v'}(y^-)\right)\\ &\quad - \left(u'(y^+)\,\overline{v}(y^+) - u'(y^-)\,\overline{v}(y^-)\right)\\ &= \det\begin{pmatrix} u(y^+) & \overline{v}(y^+)\\ u'(y^+) & \overline{v'}(y^+)\end{pmatrix} - \det\begin{pmatrix} u(y^-) & \overline{v}(y^-)\\ u'(y^-) & \overline{v'}(y^-)\end{pmatrix}\\ &= \left(\det\mathbf{A}(y) - 1\right)\det\begin{pmatrix} u(y^-) & \overline{v}(y^-)\\ u'(y^-) & \overline{v'}(y^-)\end{pmatrix} = 0, \quad \forall y \in \mathcal{Y},\end{aligned}$$

where we have used the condition $\det\mathbf{A}(y) = 1$. Hence, the operators $-\frac{d^2}{dx^2}$ and S_{q_0} with domain $\widetilde{H}^2(\Gamma)$ are symmetric operators in $L^2(\mathbb{R})$. It follows from Proposition 2 that there exists $\mu_0 > 0$ such that $S_{q_0} + \mu_0^2 : \widetilde{H}^2(\Gamma) \to L^2(\mathbb{R})$ is an isomorphism. To prove that $\mathcal{H}_{q_0} + \mu_0^2$ with domain $\widetilde{H}^2(\Gamma)$ is a self-adjoint operator in $L^2(\mathbb{R})$ we have to show that $\mathrm{Dom}\left(\left(S_{q_0} + \mu_0^2\right)^*\right) = \mathrm{Dom}\left(S_{q_0} + \mu_0^2\right)$. Since $S_{q_0} + \mu_0^2$ is a symmetric operator $\mathrm{Dom}\left(S_{q_0} + \mu_0^2\right) \subset \mathrm{Dom}\left(\left(S_{q_0} + \mu_0^2\right)^*\right)$. Assume that $u \in \mathrm{Dom}\left(\left(S_{q_0} + \mu_0^2\right)^*\right)$, then $\left(S_{q_0} + \mu_0^2\right)^* u = f \in L^2(\mathbb{R})$. Since $S_{q_0} + \mu_0^2 : \mathrm{Dom}\left(S_{q_0}\right) \to L^2(\mathbb{R})$ is an isomorphism, there exists $v \in \mathrm{Dom}\left(S_{q_0} + \mu_0^2\right)$ such that $\left(S_{q_0} + \mu_0^2\right) v = f$. Since $\mathrm{Dom}\left(S_{q_0} + \mu_0^2\right) \subset \mathrm{Dom}\left(\left(S_{q_0} + \mu_0^2\right)^*\right)$ we obtain that $\left(S_{q_0} + \mu_0^2\right)^* v = f$. Hence

$$u - v \in \ker\left(S_{q_0} + \mu_0^2\right)^* = \left(\mathrm{Im}\left(S_{q_0} + \mu_0^2\right)\right)^\perp = \{0\}.$$

Therefore, $u = v \in \mathrm{Dom}\left(S_{q_0} + \mu_0^2\right)$ and $\mathrm{Dom}\left(S_{q_0} + \mu_0^2\right) = \mathrm{Dom}\left(\left(S_{q_0} + \mu_0^2\right)^*\right)$. Thus, $S_{q_0} + \mu_0^2$ is a self-adjoint operator in $L^2(\mathbb{R})$ with domain $\mathrm{Dom}\left(S_{q_0}\right) = \widetilde{H}^2(\Gamma)$. Note that the operator of multiplication by μ_0^2 is strongly dominated by the operator S_{q_0} (see, e.g., [18, p. 73]). Hence, $\mathcal{H}_{q_0}$ with domain $\widetilde{H}^2(\Gamma)$ is a self-adjoint operator.

2.3. Fredholm Property and Essential Spectrum of Schrödinger Operators With Point Interactions

In this subsection we give the necessary and sufficient conditions of Fredholmness for Schrödinger operators $S_{q_0} : \widetilde{H}^2(\Gamma) \to L^2(\mathbb{R})$ with point interactions in terms of limit operators. We apply these results to the description of the essential spectrum of the corresponding unbounded operators $\mathcal{H}_{q_0}$. Through this subsection we assume that the sequence of points $\mathcal{Y} = \{y_j\}_{j\in\mathbb{Z}} \subset \mathbb{R}$ where the singular potential q_s is supported is periodic with respect to the group $\mathbb{G} = \ell\mathbb{Z}$, $\ell > 0$. We also assume that matrices $\mathcal{Y} \ni y \mapsto \mathbf{A}(y)$ are periodic with respect to $\mathbb{G}$.

Definition 1. *A potential* $q_0 \in L^\infty(\mathbb{R})$ *is said to be rich if for every sequence* $g = (g_m)$, $\mathbb{G} \ni g_m \to \infty$, *there exists a subsequence* $h = (h_m)$, $h_m \to \infty$, *and a limit function* $q_0^h \in L^\infty(\mathbb{R})$ *such that for every segment* $[a, b] \subset \mathbb{R}$

$$\lim_{m\to\infty} \sup_{x\in[a,b]} \left| q_0^h(x) - q_0(x + h_m) \right| = 0.$$

Definition 2. *The Schrödinger operator* $S_{q_0^h} : \widetilde{H}^2(\Gamma) \to L^2(\mathbb{R})$ *defined by*

$$S_{q_0^h} u(x) := \left(-\frac{d^2}{dx^2} + q_0^h(x) \right) u(x), \qquad x \in \Gamma,$$

with a limit function q_0^h *replacing the rich potential* q_0 *is called a limit operator of* $S_{q_0} : \widetilde{H}^2(\Gamma) \to L^2(\mathbb{R})$. *The set of all limit operators of* S_{q_0} *is denoted by* $\mathrm{Lim}\left(S_{q_0}\right)$.

Let $\varphi \in C_0^\infty(\mathbb{R})$ such that $0 \leq \varphi(x) \leq 1$, where $\varphi(x) = 1$ if $|x| \leq \frac{1}{2}$, and $\varphi(x) = 0$ if $|x| \geq 1$. Let $\varphi_R(x) = \varphi(x/R)$, and $\psi_R(x) = 1 - \varphi_R(x)$.

Theorem 3. *Let* $q_0 \in L^\infty(\mathbb{R})$ *be a rich potential, and let matrices* $\mathcal{Y} \ni y \mapsto \mathbf{A}(y)$ *be* $\mathbb{G}$*-periodic. Then* $S_{q_0} : \widetilde{H}^2(\Gamma) \to L^2(\mathbb{R})$ *is a Fredholm operator if and only if all limit operators* $S_{q_0^h} : \widetilde{H}^2(\Gamma) \to L^2(\mathbb{R})$ *are invertible.*

Proof: One can prove that the operator $S_{q_0} : \widetilde{H}^2(\Gamma) \to L^2(\mathbb{R})$ is locally Fredholm, that is for every $R > 0$ there exist operators $\mathcal{L}_R, \mathcal{R}_R \in \mathcal{B}\left(L^2(\mathbb{R}), \widetilde{H}^2(\Gamma)\right)$ such that

$$\mathcal{L}_R S_{q_0} \varphi_R = \varphi_R + T_R^{(1)}, \quad \varphi_R S_{q_0} \mathcal{R}_R = \varphi_R + T_R^{(2)},$$

where $T_R^{(1)} \in \mathcal{K}\left(\widetilde{H}^2(\Gamma)\right)$, and $T_R^{(2)} \in \mathcal{K}\left(L^2(\mathbb{R})\right)$ since S_{q_0} is an elliptic operator. Hence, in order to prove that $S_{q_0} : \widetilde{H}^2(\Gamma) \to L^2(\mathbb{R})$ is a Fredholm operator we have to study the local

invertibility of S_{q_0} at infinity, *i.e.*, we have to prove that there exists $R_0 > 0$ and operators $\mathcal{L}_{R_0}^{\infty}, \mathcal{R}_{R_0}^{\infty} \in \mathcal{B}\left(L^2(\mathbb{R}), \widetilde{H}^2(\Gamma)\right)$ such that

$$\mathcal{L}_{R_0}^{\infty} S_{q_0} \psi_{R_0} = \psi_{R_0}, \quad \psi_{R_0} S_{q_0} \mathcal{R}_{R_0}^{\infty} = \psi_{R_0}.$$

Let $\mu_0 > 0$ be such that the operator $S_{\mu_0^2} : \widetilde{H}^2(\Gamma) \to L^2(\mathbb{R})$ is an isomorphism. We set

$$\mathcal{A} = S_{q_0} S_{\mu_0^2}^{-1} : L^2(\mathbb{R}) \to L^2(\mathbb{R}).$$

It is easy to prove that $S_{q_0} : \widetilde{H}^2(\Gamma) \to L^2(\mathbb{R})$ is locally invertible at infinity if and only if $\mathcal{A}$ is locally invertible at infinity. For the study of local invertibility at infinity we use the results of the book [19], and the work [20].

Let $\phi \in C_b^{\infty}(\mathbb{R})$, and $\phi_t(x) = \phi(tx)$, $t \in \mathbb{R}$. Then it is easy to prove that

$$\lim_{t \to 0} \|[\phi_t, \mathcal{A}]\| = \lim_{t \to 0} \|\phi_t \mathcal{A} - \mathcal{A}\phi_t\| = 0,$$

that is, $\mathcal{A}$ belongs to the C^*-algebra of so-called band-dominated operators in $L^2(\mathbb{R})$ (see, e.g., [20]). We introduce the limit operators of $\mathcal{A}$ as follows. For $\mathbb{G} \ni h_m \to \infty$ let $V_{h_m} u(x) := u\left(x - h_m\right)$ be the corresponding sequence of shift operators. We say that $\mathcal{A}^h$ is a limit operator defined by the sequence $h = \left(h_m\right)$ if

$$\begin{aligned} &\left\| \left(V_{-h_m} \mathcal{A} V_{h_m} - \mathcal{A}^h \right) \varphi \right\|_{\mathcal{B}(L^2(\mathbb{R}))} \\ &= \left\| \varphi \left(V_{-h_m} \mathcal{A} V_{h_m} - \mathcal{A}^h \right) \right\|_{\mathcal{B}(L^2(\mathbb{R}))} = 0 \end{aligned} \tag{9}$$

for every $\varphi \in C_0^{\infty}(\mathbb{R})$. One can see that

$$V_{-h_m} \mathcal{A} V_{h_m} = V_{-h_m} \mathcal{H}_{q_0} V_{h_m} S_{\mu_0^2}^{-1}. \tag{10}$$

Formulas (9), (10) imply that

$$\mathcal{A}^h = S_{q_0^h} S_{\mu_0^2}^{-1}.$$

Moreover, since the potential q_0 is rich the operator $\mathcal{A}$ is rich, that is, every sequence $g = \left(g_m\right)$ of $\mathbb{G}$ tending to infinity has a subsequence $h = \left(h_m\right)$ tending to infinity that defines the limit operator $\mathcal{A}^h$. It follows from the results of Rabinovich et al. [19] and Lindner and Seidel [20] that the operator $\mathcal{A}$ is locally invertible at infinity if and only if all limit operators $\mathcal{A}^h$ are invertible. Since $S_{\mu_0^2} : \widetilde{H}^2(\Gamma) \to L^2(\mathbb{R})$ is an isomorphism, this yields the statement of the theorem.

Theorem 3 leads to the following description of the essential spectrum of operator $\mathcal{H}_{q_0}$.

Theorem 4. *Let $q_0 \in L^{\infty}(\mathbb{R})$ be a rich potential, and let the matrices $\mathcal{Y} \ni y \mapsto \mathbf{A}(y)$ be $\mathbb{G}$-periodic. Then*

$$\mathrm{sp}_{\mathrm{ess}} \mathcal{H}_{q_0} = \bigcup_{\mathcal{H}_{q_0^h} \in \mathrm{Lim}(\mathcal{H}_{q_0})} \mathrm{sp} \mathcal{H}_{q_0^h}, \tag{11}$$

where $\mathcal{H}_{q_0^h}$ is the limit operator of $\mathcal{H}_{q_0}$ defined as an unbounded operator in $L^2(\mathbb{R})$, generated by the Schrödinger operator $S_{q_0^h}$ with domain $\widetilde{H}^2(\Gamma)$.

3. SPECTRAL ANALYSIS OF PERIODIC SCHRÖDINGER OPERATORS WITH POINT INTERACTIONS

In this section we study the band-gap spectra of periodic Schrödinger operators with point interactions by using the Floquet transform (see e.g., [21]). We also analyze the case when the regular potential q_0 is perturbed by a slowly oscillating at infinity term by means of the limit operators method, and provide expressions for the essential spectrum of corresponding Schrödinger operator.

3.1. Periodic Schrödinger Operators With Point Interactions

From now on we will assume that:

1. the sequence of points $\mathcal{Y} = \left\{y_j\right\}_{j \in \mathbb{Z}} \subset \mathbb{R}$ on which the singular potential q_s is supported is periodic with respect to the group $\mathbb{G} = \ell\mathbb{Z}$, $\ell > 0$;
2. the matrices $\mathbf{A}(y) = \left(a_{ij}(y)\right)_{i,j=1}^2$ are periodic with respect to the group $\mathbb{G}$, that is, $\mathbf{A}(y+g) = \mathbf{A}(y)$ for every $g \in \mathbb{G}$ and $y \in \mathcal{Y}$. The entries $a_{ij} \in l^{\infty}(\mathcal{Y})$ of the matrices are such that $\det \mathbf{A}(y) = 1$ for every $y \in \mathcal{Y}$; and
3. the potential q_0 is a real-valued, piecewise continuous function, periodic with respect to the group $\mathbb{G}$.

Let $\Gamma_0 := [0, \ell)$, and $\mathbb{B} = [-\pi/\ell, \pi/\ell)$ be the reciprocal unit cell (also known as Brillouin zone) of Γ_0. Let $\mathcal{Y}_0 := \mathcal{Y} \cap \Gamma_0 = \left\{y_1, \cdots, y_n\right\}$ be the set of points of discontinuity inside Γ_0, which satisfy $0 < y_1 < \cdots < y_n < \ell$. We also assume that the finite jumps $\left[q_0\right]_{y_j}$, not necessarily zero, are well-defined.

From conditions (1–3) and Theorem 3 it follows that the operator $\mathcal{H}_{q_0}$ with domain $\widetilde{H}^2(\Gamma)$ is self-adjoint in $L^2(\mathbb{R})$. Moreover, the operator S_{q_0} is invariant with respect to the shifts on the elements of the group $\mathbb{G}$, that is

$$\begin{aligned} V_g S_{q_0} u(x) &= -\frac{d^2 u(x+g)}{dx^2} + q_0(x+g)\, u(x+g) \\ &= -\frac{d^2 u(x+g)}{dx^2} + q_0(x)\, u(x+g) = S_{q_0} V_g u(x), \end{aligned}$$

for every $g \in \mathbb{G}$. Since $V_g S_{q_0} = S_{q_0} V_g$, and from (11), it yields that $\mathrm{sp}_{\mathrm{ess}} \mathcal{H}_{q_0} = \mathrm{sp} \mathcal{H}_{q_0}$, and $\mathrm{sp}_{\mathrm{dis}} \mathcal{H}_{q_0} = \emptyset$. In addition, the operator S_{q_0} is semi-bounded from below, that is

$$\left\langle S_{q_0} u, u \right\rangle \geq m_{q_0} \|u\|_{L^2(\mathbb{R})}^2,$$

where $m_{q_0} := \inf_{x \in \mathbb{R}} q_0(x)$. This implies that

$$\mathrm{sp} \mathcal{H}_{q_0} \subset \left[m_{q_0}, +\infty\right).$$

We introduce the Hilbert space $H := L^2\left(\Gamma_0, L^2(\mathbb{B})\right)$ of vector-valued functions with components in $L^2(\Gamma_0)$, which is equipped by the norm

$$\|u\|_H = \left(\int_{\Gamma_0} \|u(x,\cdot)\|^2_{L^2(\mathbb{B})}\, \mathrm{d}x\right)^{1/2}.$$

The Floquet transform is the map $\mathcal{F}: L^2(\mathbb{R}) \to H$ defined for functions f that decay sufficiently fast by

$$\left(\mathcal{F}f\right)(x,\theta) = \widetilde{f}(x,\theta) := \frac{1}{\sqrt{2\pi}} \sum_{\alpha\in\mathbb{Z}} f(x-\alpha\ell)\, e^{\mathrm{i}\alpha\theta},\ x\in\mathbb{R},\ \theta\in\mathbb{B},$$

where the parameter θ is often called the quasi-momentum. The Floquet transform is an isometry from $L^2(\mathbb{R})$ to H, whose inverse is given by

$$\left(\mathcal{F}^{-1}\widetilde{f}\right)(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{B}} \widetilde{f}(x,\theta)\, \mathrm{d}\theta.$$

Let us consider the problem

$$\mathcal{H}_{q_0} u(x) = \lambda u(x), \quad u \in \widetilde{H}^2(\Gamma), \tag{12}$$

where $\lambda \in \mathbb{R}$ is the spectral parameter. The Floquet transform applied to (12) gives a spectral problem depending on the parameter $\theta \in \mathbb{B}$, defined by the differential equation

$$S_{q_0}\widetilde{u}(x,\theta) = \lambda\widetilde{u}(x,\theta), \quad x\in(0,\ell)\setminus\mathcal{Y}_0,\ \theta\in\mathbb{B},$$

with the interaction conditions at the discontinuity points

$$\begin{pmatrix} \widetilde{u}\left(y^+,\theta\right) \\ \widetilde{u}'_x\left(y^+,\theta\right)\end{pmatrix} = \mathbf{A}(y)\begin{pmatrix} \widetilde{u}\left(y^-,\theta\right) \\ \widetilde{u}'_x\left(y^-,\theta\right)\end{pmatrix}, \quad y\in\mathcal{Y}_0,$$

and the quasi-periodic conditions

$$\widetilde{u}(\ell,\theta) = e^{\mathrm{i}\theta\ell}\widetilde{u}(0,\theta), \quad \widetilde{u}'_x(\ell,\theta) = e^{\mathrm{i}\theta\ell}\widetilde{u}'_x(0,\theta).$$

The operator $S_{q_0} = \mathcal{F}S_{q_0}\mathcal{F}^{-1}$ is represented as the orthogonal sum

$$S_{q_0} = \mathcal{F}S_{q_0}\mathcal{F}^{-1} = \bigoplus_{\theta\in\mathbb{B}} S^\theta_{q_0}, \tag{13}$$

where

$$S^\theta_{q_0} u(x,\theta) := -\frac{d^2u(x,\theta)}{dx^2} + q_0(x)\,u(x,\theta), \quad x\in(0,\ell)\setminus\mathcal{Y}_0.$$

For each $\theta\in\mathbb{B}$, the operator $S^\theta_{q_0}$ defines an unbounded operator $\mathcal{H}^\theta_{q_0}$ in $L^2(\Gamma_0)$ with domain $\mathrm{Dom}\left(\mathcal{H}^\theta_{q_0}\right) = \widetilde{H}^2(\Gamma_0\setminus\mathcal{Y}_0)$, where

$$\begin{aligned}&\widetilde{H}^2(\Gamma_0\setminus\mathcal{Y}_0)\\ &= \left\{u\in H^2(\Gamma_0\setminus\mathcal{Y}_0):\ \begin{pmatrix} u\left(y^+,\theta\right) \\ u'_x\left(y^+,\theta\right)\end{pmatrix} = \mathbf{A}(y)\begin{pmatrix} u\left(y^-,\theta\right) \\ u'_x\left(y^-,\theta\right)\end{pmatrix}, y\in\mathcal{Y}_0,\right.\\ &\left. u(\ell,\theta) = e^{\mathrm{i}\theta\ell}u(0,\theta),\ u'_x(\ell,\theta) = e^{\mathrm{i}\theta\ell}u'_x(0,\theta),\ \theta\in\mathbb{B}\right\}.\end{aligned}$$

Operators $\mathcal{H}^\theta_{q_0}$, $\theta\in\mathbb{B}$, with domain $\widetilde{H}^2(\Gamma_0\setminus\mathcal{Y}_0)$ have discrete spectra

$$\mathrm{sp}\mathcal{H}^\theta_{q_0} = \left\{\lambda_1(\theta) < \lambda_2(\theta) < \cdots < \lambda_j(\theta) < \cdots\right\},$$

where $\lambda_j(\theta)$ are continuous functions on $\mathbb{B}$. Expression (13) implies that

$$\mathrm{sp}\mathcal{H}_{q_0} = \bigcup_{\theta\in\mathbb{B}} \mathrm{sp}\mathcal{H}^\theta_{q_0}. \tag{14}$$

If the image of the Brillouin zone $\mathbb{B}$ under λ_j is $\left[a_j, b_j\right]$, $a_j \le b_j$, $j\in\mathbb{N}$, then formula (14) gives

$$\mathrm{sp}\mathcal{H}_{q_0} = \bigcup_{j=1}^{\infty}\left[a_j, b_j\right], \tag{15}$$

that is, the spectrum of Schrödinger operator $\mathcal{H}_{q_0}$ with $\mathbb{G}$-periodic potential q_0 involving point interactions has a band-gap structure.

3.2. Spectral Analysis of Periodic Schrödinger Operators With Point Interactions

For each $\theta\in\mathbb{B}$ we define the spectral problem

$$\mathcal{H}^\theta_{q_0} u(x,\theta) = \lambda(\theta)\,u(x,\theta), \quad u\in\widetilde{H}^2(\Gamma_0\setminus\mathcal{Y}_0).$$

Solutions of this problem are sought in the form

$$u(x,\theta;\lambda) = C_1(\theta,\lambda)\,\varphi_1(x,\lambda) + C_2(\theta,\lambda)\,\varphi_2(x,\lambda),$$

where C_1, C_2 are arbitrary coefficients, and φ_1, φ_2 are linearly independent solutions of the Schrödinger equation

$$S_{q_0}u = \lambda u, \quad x\in(0,\ell)\setminus\mathcal{Y}_0$$

satisfying the interaction conditions

$$\begin{pmatrix} u\left(y^+\right) \\ u'_x\left(y^+\right)\end{pmatrix} = \mathbf{A}(y)\begin{pmatrix} u\left(y^-\right) \\ u'_x\left(y^-\right)\end{pmatrix}, \quad y\in\mathcal{Y}_0,$$

as well as the initial conditions

$$\varphi_1(0,\lambda) = 1, \quad (\varphi_1)'_x(0,\lambda) = 0, \tag{16a}$$
$$\varphi_2(0,\lambda) = 0, \quad (\varphi_2)'_x(0,\lambda) = 1. \tag{16b}$$

By the Liouville identity, the Wronskian of φ_1 and φ_2 satisfies

$$\begin{aligned}&\det\begin{pmatrix} \varphi_1(0,\lambda) & \varphi_2(0,\lambda) \\ (\varphi_1)'_x(0,\lambda) & (\varphi_2)'_x(0,\lambda)\end{pmatrix}\\ &= \det\begin{pmatrix} \varphi_1(x,\lambda) & \varphi_2(x,\lambda) \\ (\varphi_1)'_x(x,\lambda) & (\varphi_2)'_x(x,\lambda)\end{pmatrix} = 1,\\ &\forall x\in[0,\ell]\setminus\mathcal{Y}_0.\end{aligned}$$

From the quasi-periodic property

$$u(\ell,\theta) = e^{\mathrm{i}\theta\ell}u(0,\theta), \quad u'_x(\ell,\theta) = e^{\mathrm{i}\theta\ell}u'_x(0,\theta)$$

we obtain the following system of equations

$$C_1(\theta,\lambda)\,\varphi_1(\ell,\lambda)+C_2(\theta,\lambda)\,\varphi_2(\ell,\lambda)=e^{\mathrm{i}\theta\ell}C_1(\theta,\lambda), \tag{17a}$$

$$C_1(\theta,\lambda)\,(\varphi_1)'_x(\ell,\lambda)+C_2(\theta,\lambda)\,(\varphi_2)'_x(\ell,\lambda)=e^{\mathrm{i}\theta\ell}C_2(\theta,\lambda), \tag{17b}$$

with C_1, C_2 as unknowns. System (17) implies that $\left(C_1(\theta,\lambda)\ C_2(\theta,\lambda)\right)^{\mathsf{T}}$ is an eigenvector of the monodromy matrix

$$\mathbf{M}(\lambda)=\begin{pmatrix}\varphi_1(\ell,\lambda) & \varphi_2(\ell,\lambda)\\ (\varphi_1)'_x(\ell,\lambda) & (\varphi_2)'_x(\ell,\lambda)\end{pmatrix}$$

associated to the eigenvalue $\mu:=e^{\mathrm{i}\theta\ell}$. In order for system (17) to possess non-trivial solutions its determinant must vanish, that is

$$\det\begin{pmatrix}\varphi_1(\ell,\lambda)-\mu & \varphi_2(\ell,\lambda)\\ (\varphi_1)'_x(\ell,\lambda) & (\varphi_2)'_x(\ell,\lambda)-\mu\end{pmatrix}=0$$

This leads to the dispersion equation

$$\mu^2-2\mu D(\lambda)+1=0, \tag{18}$$

where

$$D(\lambda):=\frac{1}{2}\left(\varphi_1(\ell,\lambda)+(\varphi_2)'_x(\ell,\lambda)\right).$$

Equation (18) has solutions of the form $\mu:=e^{\mathrm{i}\theta\ell}$, $\theta\in\mathbb{B}$, if and only if $|D(\lambda)|\le 1$. Hence, the spectrum of $\mathcal{H}_{q_0}$ is given by

$$\mathrm{sp}\mathcal{H}_{q_0}=\{\lambda\in\mathbb{R}:\,|D(\lambda)|\le 1\},$$

and the edges of the spectral bands of $\mathrm{sp}\mathcal{H}_{q_0}$ are solutions $\lambda_{\mathrm{edge}}\in\mathbb{R}$ of the equation

$$\left|D\left(\lambda_{\mathrm{edge}}\right)\right|=1.$$

3.3. Periodic Potentials Perturbed by Slowly Oscillating at Infinity Terms

A function $a\in L^\infty(\mathbb{R})$ is slowly oscillating at infinity if the limit

$$\lim_{x\to\infty}\sup_{y\in K}\left|a(x+y)-a(x)\right|=0$$

holds for every compact set $K\subset\mathbb{R}$. We denote by $\mathrm{SO}(\mathbb{R})$ the class of such functions. One can prove (see, e.g., [19, Chap. 3.1]) that all limit functions a^h of $a\in\mathrm{SO}(\mathbb{R})$ defined by the sequence $\mathbb{G}\ni h_m\to\infty$ are real constants.

Let us consider a Schrödinger operator $\mathcal{H}_q:\widetilde{H}^2(\Gamma)\to L^2(\mathbb{R})$ with a perturbed potential $q=q_0+q_1$ consisting of a periodic part $q_0\in L^\infty(\mathbb{R})$ satisfying conditions (3), and a real-valued perturbation $q_1\in\mathrm{SO}(\mathbb{R})$. The result of Theorem 4 can be used for analyzing the essential spectrum of $\mathcal{H}_q$. Note that the spectrum of operator $\mathcal{H}_{q_0}$ has a band-gap structure according to (15). The limit operators of $\mathcal{H}_q=\mathcal{H}_{q_0+q_1}$ are of the form $\mathcal{H}_{q^h}=\mathcal{H}_{q_0+q_1^h}$, where $q_1^h\in\mathbb{R}$. Therefore

$$\mathrm{sp}\mathcal{H}_{q_0+q_1^h}=\bigcup_{j=1}^{\infty}\left[a_j+q_1^h,b_j+q_1^h\right].$$

On considering formula (11) and previous expression we obtain the essential spectrum of perturbed operator $\mathcal{H}_q=\mathcal{H}_{q_0+q_1}$, that is

$$\mathrm{sp}_{\mathrm{ess}}\mathcal{H}_q=\bigcup_{j=1}^{\infty}\left[a_j+m_{q_1}^{\infty},b_j+M_{q_1}^{\infty}\right], \tag{19}$$

where

$$m_{q_1}^{\infty}:=\liminf_{x\to\infty}q_1(x),\quad M_{q_1}^{\infty}:=\limsup_{x\to\infty}q_1(x).$$

Formula (19) implies that some spectral bands of $\mathrm{sp}_{\mathrm{ess}}\mathcal{H}_q$ may overlap depending on the intensity of the perturbation q_1. Let $\left(b_l+M_{q_1}^{\infty},a_{l+1}+m_{q_1}^{\infty}\right)$, $l\in\mathbb{N}$, be a gap of $\mathrm{sp}_{\mathrm{ess}}\mathcal{H}_q$, hence if the relation

$$M_{q_1}^{\infty}-m_{q_1}^{\infty}>a_{l+1}-b_l \tag{20}$$

holds the gap will disappear due to the merging of the adjacent bands. If condition (20) is satisfied for all $l\in\mathbb{N}$, all spectral gaps of $\mathrm{sp}_{\mathrm{ess}}\mathcal{H}_q$ will disappear resulting a continuous spectrum, that is

$$\mathrm{sp}_{\mathrm{ess}}\mathcal{H}_q=\left[a_1+m_{q_1}^{\infty},+\infty\right),\ \text{and}\ \mathrm{sp}_{\mathrm{dis}}\mathcal{H}_q\subset\left[m_{q_0},a_1+m_{q_1}^{\infty}\right).$$

4. DISPERSION EQUATION FOR PERIODIC SCHRÖDINGER OPERATORS WITH POINT INTERACTIONS

In this section we determine the function $D(\lambda)$ from a set of monodromy matrices specified at the points where the singular potential is supported in the fundamental domain Γ_0. We also apply the spectral parameter power series method [10] to derive a numerical method for calculating the spectral bands of Schrödinger operators $\mathcal{H}_{q_0}$ with arbitrary regular potentials q_0 satisfying certain smoothness conditions.

4.1. Calculation of Function $D(\lambda)$ in Terms of Monodromy Matrices

We begin by determining a general solution of the equation

$$-\frac{d^2u(x)}{dx^2}+q_0(x)\,u(x)=\lambda u,\qquad x\in(0,\ell)\setminus\mathcal{Y}_0, \tag{21}$$

satisfying the interaction conditions

$$\begin{pmatrix}u\left(y_j^+\right)\\ u'\left(y_j^+\right)\end{pmatrix}=\mathbf{A}\left(y_j\right)\begin{pmatrix}u\left(y_j^-\right)\\ u'\left(y_j^-\right)\end{pmatrix},$$

$$\mathbf{A}\left(y_j\right)=\begin{pmatrix}\frac{4-\alpha_j\beta_j}{4+\alpha_j\beta_j} & \frac{-4\beta_j}{4+\alpha_j\beta_j}\\ \frac{4\alpha_j}{4+\alpha_j\beta_j} & \frac{4-\alpha_j\beta_j}{4+\alpha_j\beta_j}\end{pmatrix},\ \alpha_j\beta_j\neq-4,$$

at the points of discontinuity $y_j \in \mathcal{Y}_0$ $(j = 1, \cdots, n)$. By abusing the notation, we set $y_0 \equiv 0$, and $y_{n+1} \equiv \ell$. The interval between two adjacent points of discontinuity y_j, y_{j+1} is denoted by $e_j = (y_j, y_{j+1})$ $(j = 0, \cdots, n)$. Let $\phi_{1,j}$, $\phi_{2,j}$ $(j = 0, \cdots, n)$ be a pair of linearly independent solutions of Equation (21) on the interval e_j, which satisfy the Cauchy conditions

$$\phi_{1,j}(y_j) = 1, \qquad \phi_{2,j}(y_j) = 0, \tag{22a}$$
$$\phi'_{1,j}(y_j) = 0, \qquad \phi'_{2,j}(y_j) = 1. \tag{22b}$$

From these solutions we define the monodromy matrices

$$\mathbf{M}_{j,j+1} := \begin{pmatrix} \phi_{1,j}(y_{j+1}) & \phi_{2,j}(y_{j+1}) \\ \phi'_{1,j}(y_{j+1}) & \phi'_{2,j}(y_{j+1}) \end{pmatrix}, \ j = 0, \cdots, n.$$

Let $u_{e_j} = u|_{e_j}$ $(j = 0, \cdots, n)$ be the restriction of solution u of Equation (21) on e_j, which can be written as

$$u_{e_j}(x) = u_{e_j}(y_j)\,\phi_{1,j}(x) + u'_{e_j}(y_j)\,\phi_{2,j}(x), \quad x \in e_j.$$

Hence, on the full interval $[0, \ell)$, a general solution of Equation (21) is given by the piecewise continuous function

$$u(x) = \begin{cases} u_{e_0}(y_0)\,\phi_{1,0}(x) + u'_{e_0}(y_0)\,\phi_{2,0}(x), & 0 \le x < y_1, \\ u_{e_1}(y_1)\,\phi_{1,1}(x) + u'_{e_1}(y_1)\,\phi_{2,1}(x), & y_1 < x < y_2, \\ \vdots & \vdots \\ u_{e_n}(y_n)\,\phi_{1,n}(x) + u'_{e_n}(y_n)\,\phi_{2,n}(x), & y_n < x < \ell, \end{cases}$$

where the coefficients $u_{e_j}(y_j)$ and $u'_{e_j}(y_j)$ $(j = 1, \cdots, n)$ are given in a matrix form by

$$\begin{aligned} &\begin{pmatrix} u_{e_j}(y_j) \\ u'_{e_j}(y_j) \end{pmatrix} = \mathbf{A}_j \begin{pmatrix} u_{e_{j-1}}(y_j) \\ u'_{e_{j-1}}(y_j) \end{pmatrix} \\ &= \mathbf{A}_j \mathbf{M}_{j-1,j} \cdots \mathbf{A}_1 \mathbf{M}_{0,1} \begin{pmatrix} u_{e_0}(y_0) \\ u'_{e_0}(y_0) \end{pmatrix}, \quad j = 1, \cdots, n. \end{aligned} \tag{23}$$

The restriction u_{e_n} and its derivative u'_{e_n} evaluated at $x = \ell$ gives the matrix relation

$$\begin{pmatrix} u_{e_n}(\ell) \\ u'_{e_n}(\ell) \end{pmatrix} = \mathbf{M}_{n,n+1} \begin{pmatrix} u_{e_n}(y_n) \\ u'_{e_n}(y_n) \end{pmatrix}. \tag{24}$$

By plugging formulas (23) and (24) we obtain the expression

$$\begin{pmatrix} u(\ell;\lambda) \\ u'(\ell;\lambda) \end{pmatrix} = \mathbf{T}(\lambda) \begin{pmatrix} u(0;\lambda) \\ u'(0;\lambda) \end{pmatrix} = \begin{pmatrix} T_{11}(\lambda) & T_{12}(\lambda) \\ T_{21}(\lambda) & T_{22}(\lambda) \end{pmatrix} \begin{pmatrix} u(0;\lambda) \\ u'(0;\lambda) \end{pmatrix},$$

where $\mathbf{T} := \mathbf{M}_{n,n+1}\mathbf{A}_n\mathbf{M}_{n-1,n} \cdots \mathbf{A}_2\mathbf{M}_{1,2}\mathbf{A}_1\mathbf{M}_{0,1}$ is a 2×2-matrix called the transmission matrix.

Therefore, solutions φ_1 and φ_2 that fulfill conditions (16) satisfy the matrix equations

$$\begin{pmatrix} \varphi_1(\ell,\lambda) \\ (\varphi_1)'_x(\ell,\lambda) \end{pmatrix} = \mathbf{T}(\lambda) \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} T_{11}(\lambda) \\ T_{21}(\lambda) \end{pmatrix},$$
$$\begin{pmatrix} \varphi_2(\ell,\lambda) \\ (\varphi_2)'_x(\ell,\lambda) \end{pmatrix} = \mathbf{T}(\lambda) \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} T_{12}(\lambda) \\ T_{22}(\lambda) \end{pmatrix},$$

thereby the function $D(\lambda)$ can be written in the form

$$D(\lambda) = \frac{1}{2}\left(T_{11}(\lambda) + T_{22}(\lambda)\right). \tag{25}$$

4.2. Some Solvable Models With Periodic Singular Potentials

If the potential q_0 vanishes identically on $\mathbb{R}$ it is possible to obtain exact solutions of Equation (21) on the interval $e_j = (y_j, y_{j+1})$. One can see that $\phi_{1,j}(x,\lambda) = \cos\sqrt{\lambda}(x - y_j)$, $\phi_{2,j}(x,\lambda) = \frac{1}{\sqrt{\lambda}}\sin\sqrt{\lambda}(x - y_j)$ are solutions of the Schrödinger equation for a free-particle

$$-\frac{d^2u(x)}{dx^2} = \lambda u, \quad x \in e_j,\ j = 0, 1 \cdots, n,$$

with energy λ, which satisfy Cauchy conditions (22). In this case, monodromy matrices read

$$\mathbf{M}_{j,j+1}(\lambda) = \begin{pmatrix} \cos\sqrt{\lambda}\,|e_j| & \frac{1}{\sqrt{\lambda}}\sin\sqrt{\lambda}\,|e_j| \\ -\sqrt{\lambda}\sin\sqrt{\lambda}\,|e_j| & \cos\sqrt{\lambda}\,|e_j| \end{pmatrix}, \ j = 0, \cdots, n.$$

Periodic Potential With Only δ-Distributions

The periodic potential involving only Dirac delta distributions

$$q_\delta(x) = \sum_{n\in\mathbb{Z}} \alpha\delta\left(x - \left(n + \frac{1}{2}\right)\ell\right), \quad \alpha \in \mathbb{R} \tag{26}$$

defines at each singular point $y \in \mathcal{Y}$ the interaction matrix

$$\mathbf{A}_\alpha(y) = \begin{pmatrix} 1 & 0 \\ \alpha & 1 \end{pmatrix}. \tag{27}$$

Let $\mathcal{H}_\delta$ be the Hamiltonian defined by the ℓ-periodic potential $q_\delta(x)$. In this case $\mathcal{Y}_0 = \{\ell/2\}$, that is, $y_0 = 0$, $y_1 = \ell/2$, and $y_2 = \ell$, thereby the transmission matrix reads

$$\begin{aligned} &\mathbf{T}_\delta(\lambda) = \mathbf{M}_{1,2}(\lambda)\,\mathbf{A}_\alpha\mathbf{M}_{0,1}(\lambda) \\ &= \begin{pmatrix} \cos\ell\sqrt{\lambda} + \frac{\alpha}{2\sqrt{\lambda}}\sin\ell\sqrt{\lambda} & \frac{1}{\sqrt{\lambda}}\sin\ell\sqrt{\lambda} + \frac{\alpha}{\lambda}\sin^2\ell\sqrt{\lambda}/2 \\ \alpha\cos^2\ell\sqrt{\lambda}/2 - \sqrt{\lambda}\sin\ell\sqrt{\lambda} & \cos\ell\sqrt{\lambda} + \frac{\alpha}{2\sqrt{\lambda}}\sin\ell\sqrt{\lambda} \end{pmatrix}, \end{aligned}$$

hence, the spectrum $\mathrm{sp}\mathcal{H}_\delta$ of Hamiltonian $\mathcal{H}_\delta$ consists of $\lambda \in \mathbb{R}$ satisfying

$$-1 \le \cos\ell\sqrt{\lambda} + \frac{\alpha}{2\sqrt{\lambda}}\sin\ell\sqrt{\lambda} \le 1. \tag{28}$$

This is the so-called Kronig-Penney model (see [1, 2] and [4, §III.2.3]) that describes the non-relativistic interaction of electrons in a fixed crystal lattice, with ions represented by δ-distributions.

Periodic Potential With Only δ'-Distributions

Consider the periodic singular potential

$$q_{\delta'}(x) = \sum_{n\in\mathbb{Z}} \beta\delta'\left(x - \left(n + \frac{1}{2}\right)\ell\right), \quad \beta \in \mathbb{R}$$

with the following matrix

$$\mathbf{A}_\beta(y) = \begin{pmatrix} 1 & -\beta \\ 0 & 1 \end{pmatrix}$$

defined at the each singular point $y \in \mathcal{Y}$. Like in the previous case only one point interaction lies inside the fundamental domain Γ_0, *i.e.*, $\mathcal{Y}_0 = \{\ell/2\}$. Let $\mathcal{H}_{\delta'}$ be the Hamiltonian defined by the periodic potential $q_{\delta'}(x)$. The corresponding transmission matrix is

$$\begin{aligned}&\mathbf{T}_{\delta'}(\lambda) = \mathbf{M}_{1,2}(\lambda)\,\mathbf{A}_\beta \mathbf{M}_{0,1}(\lambda)\\ &= \begin{pmatrix} \cos \ell\sqrt{\lambda} + \frac{\beta}{2}\sqrt{\lambda}\sin \ell\sqrt{\lambda} & \frac{1}{\sqrt{\lambda}}\sin \ell\sqrt{\lambda} - \beta\cos^2 \ell\sqrt{\lambda}/2 \\ -\sqrt{\lambda}\sin \ell\sqrt{\lambda} - \beta\lambda\sin^2 \ell\sqrt{\lambda}/2 & \cos \ell\sqrt{\lambda} + \frac{\beta}{2}\sqrt{\lambda}\sin \ell\sqrt{\lambda} \end{pmatrix}.\end{aligned}$$

Hence, the spectrum $\mathrm{sp}\mathcal{H}_{\delta'}$ of Hamiltonian $\mathcal{H}_{\delta'}$ consists of $\lambda \in \mathbb{R}$ satisfying

$$-1 \le \cos \ell\sqrt{\lambda} + \frac{\beta}{2}\sqrt{\lambda}\sin \ell\sqrt{\lambda} \le 1.$$

This is the analogous of the Kronig-Penney relation (28), [4, Chap. III.3].

The analysis of problems involving δ'-interactions has gained interest over the years [22–24]. In particular, the spectral analysis of Wannier-Stark Hamiltonians including a countable set of δ'-interactions lead to models for describing high-energy scatterers with vanishing transmission amplitudes as the wave-number $k \to \infty$ (see, e.g., [25–29]).

4.3. Spectral Parameter Power Series Method for the Calculation of Function $D(\lambda)$

In previous subsection it was defined a set of monodromy matrices for the points $\mathcal{Y}_0 \cup \{0\}$ from which a transmission matrix $\mathbf{T}$ is defined. This leads to a neat expression for the function $D(\lambda)$, defined in (25). Given a potential q_0 with discontinuities at the points $\mathcal{Y}_0$, obtaining solutions $\phi_{1,j}$, $\phi_{2,j}$ $(j = 0, \cdots, n)$ of Schrödinger equation (21) in the intervals e_j $(j = 0, \cdots, n)$ could be a challenging task. However, it is always possible to apply some numerical method for calculating approximations $\widetilde{\phi}_{1,j}$, $\widetilde{\phi}_{2,j}$ of the solutions. Nonetheless, if the potential q_0 satisfies certain smoothness conditions it is possible to obtain exact solutions of the equation in the form of power series of the spectral parameter. Here we employ the SPPS method [10, 30] for constructing the entries of transmission matrix $\mathbf{T}$ from which we construct function $D(\lambda)$.

Let $u_{0,j}$ be a particular solution of the equation

$$-\frac{d^2 u_{0,j}(x)}{dx^2} + q_{0,j}(x)\,u_{0,j}(x) = 0, \qquad x \in e_j,$$

such that $u_{0,j}^2, 1/u_{0,j}^2 \in C(\overline{e_j})$, where $q_{0,j} := q_0\big|_{e_j}$ $(j = 0, \cdots, n)$ is the restriction of potential q_0 on the interval e_j. Then a general solution of (21) on e_j $(j = 0, \cdots, n)$ has the form

$$u_j(x) = c_1 u_{1,j}(x) + c_2 u_{2,j}(x), \qquad x \in e_j,$$

where c_1, c_2 are arbitrary coefficients,

$$\begin{aligned} u_{1,j}(x) &= u_{0,j}(x)\sum_{k=0}^{\infty}\lambda^k \widetilde{X}_j^{(2k)}(x), \\ u_{2,j}(x) &= u_{0,j}(x)\sum_{k=0}^{\infty}\lambda^k X_j^{(2k+1)}(x), \end{aligned} \tag{29}$$

with the functions $\widetilde{X}_j^{(n)}$, $X_j^{(n)}$ defined by the recursive integration

$$\widetilde{X}_j^{(0)} \equiv 1, \quad \widetilde{X}_j^{(n)}(x) = \begin{cases} \displaystyle\int_{y_j}^{x} \widetilde{X}_j^{(n-1)}(s)\,u_{0,j}^2(s)\,\mathrm{d}s, & n \text{ odd}, \\ \displaystyle -\int_{y_j}^{x} \widetilde{X}_j^{(n-1)}(s)\,\frac{1}{u_{0,j}^2(s)}\mathrm{d}s, & n \text{ even}, \end{cases} \tag{30a}$$

$$X_j^{(0)} \equiv 1, \quad X_j^{(n)}(x) = \begin{cases} \displaystyle -\int_{y_j}^{x} X_j^{(n-1)}(s)\,\frac{1}{u_{0,j}^2(s)}\mathrm{d}s, & n \text{ odd}, \\ \displaystyle\int_{y_j}^{x} X_j^{(n-1)}(s)\,u_{0,j}^2(s)\,\mathrm{d}s, & n \text{ even}. \end{cases} \tag{30b}$$

Moreover, series (29) converge uniformly on $\overline{e_j}$. From the recursive integration procedure we deduce that solutions $u_{1,j}$, $u_{2,j}$ satisfy the conditions

$$\begin{aligned} u_{1,j}(y_j) &= u_{0,j}(y_j), \quad & u'_{1,j}(y_j) &= u'_{0,j}(y_j), \\ u_{2,j}(y_j) &= 0, & u'_{2,j}(y_j) &= \frac{-1}{u_{0,j}(y_j)}. \end{aligned}$$

We can see that the following solutions

$$\begin{aligned} \phi_{1,j}(x) &= \frac{1}{u_{0,j}(y_j)}u_{1,j}(x) + u'_{0,j}(y_j)\,u_{2,j}(x), \\ \phi_{2,j}(x) &= -u_{0,j}(y_j)\,u_{2,j}(x) \end{aligned}$$

fulfill conditions (22). Hence, the monodromy matrices can be calculated from the matrix expressions

$$\mathbf{M}_{j,j+1}(\lambda) = \mathbf{V}_j(\lambda)\,\mathbf{U}_j, \quad j = 0, \cdots, n,$$

where

$$\begin{aligned} \mathbf{U}_j &:= \begin{pmatrix} \frac{1}{u_{0,j}(y_j)} & 0 \\ u'_{0,j}(y_j) & -u_{0,j}(y_j) \end{pmatrix}, \quad \text{and} \\ \mathbf{V}_j(\lambda) &:= \begin{pmatrix} u_{1,j}(y_{j+1};\lambda) & u_{2,j}(y_{j+1};\lambda) \\ u'_{1,j}(y_{j+1};\lambda) & u'_{2,j}(y_{j+1};\lambda) \end{pmatrix} \; j = 0, \cdots, n. \end{aligned}$$

In the numerical implementation of the problem, power series (29) should be truncated up to a finite number of terms. Let $\widetilde{u}_{1,j}$, $\widetilde{u}_{2,j}$ be the truncated versions of $u_{1,j}$, $u_{2,j}$, respectively, which are given by the sums

$$\begin{aligned} \widetilde{u}_{1,j}(x) &= u_{0,j}(x)\sum_{k=0}^{N}\lambda^k \widetilde{X}_j^{(2k)}(x), \\ \widetilde{u}_{2,j}(x) &= u_{0,j}(x)\sum_{k=0}^{N}\lambda^k X_j^{(2k+1)}(x). \end{aligned}$$

From these approximate solutions we construct approximate matrices $\widetilde{\mathbf{V}}_j(\lambda)$ $(j = 0, \cdots, n)$, and approximate monodromy matrices as follows

$$\widetilde{\mathbf{M}}_{j,j+1}(\lambda) = \widetilde{\mathbf{V}}_j(\lambda)\,\mathbf{U}_j, \quad j = 0, \cdots, n,$$

from which we obtain an approximation of the transmission matrix

$$\widetilde{\mathbf{T}} := \widetilde{\mathbf{M}}_{n,n+1}\mathbf{A}_n\widetilde{\mathbf{M}}_{n-1,n}\cdots\mathbf{A}_2\widetilde{\mathbf{M}}_{1,2}\mathbf{A}_1\widetilde{\mathbf{M}}_{0,1},$$

thereby, function $D(\lambda)$ is approximated by

$$\widetilde{D}(\lambda) = \frac{1}{2}\left(\widetilde{T}_{11}(\lambda) + \widetilde{T}_{22}(\lambda)\right). \tag{31}$$

Regarding the accuracy of approximate solutions $\widetilde{u}_{1,j}$, $\widetilde{u}_{2,j}$, a rough estimation of the tail of $u_{1,j}$ is given by (see [10])

$$\left|u_{1,j} - \widetilde{u}_{1,j}\right| = \max\left|u_{0,j}\right|\left|\cosh\sqrt{\zeta_j} - \sum_{k=0}^{N}\frac{\zeta_j^k}{(2k)!}\right|,$$

where

$$\zeta_j := |\lambda|\left(\max\left|u_{0,j}^2\right|\right)\left(\max\left|\frac{1}{u_{0,j}^2}\right|\right)\left|y_{j+1} - y_j\right|^2.$$

The corresponding estimation of the tail of $u_{2,j}$ involves the tail of the function $\sinh\sqrt{\zeta_j}$. According to these expressions, the error associated to $\widetilde{u}_{1,j}$ mainly depends on the value of the spectral parameter λ, and on the length of the interval e_j. If a number N of terms does not provides the required accuracy, the interval e_j can be subdivided, and the resulting initial value problems should be sequentially solved. The particular solution $u_{0,j}$ also influences the accuracy of $\widetilde{u}_{1,j}$, $\widetilde{u}_{2,j}$. This solution can be obtained by means of numerical techniques, or by the SPPS method itself [10].

Given that the error increases for the large values of λ, a shifting of the spectral parameter (29) can be implemented for reducing the error. More precisely, if $u_{0,j}$ is a solution of the equation

$$-\frac{d^2u_{0,j}(x)}{dx^2} + q_{0,j}(x)\,u_{0,j}(x) = \lambda_0 u_{0,j}(x) \qquad x \in e_j,$$

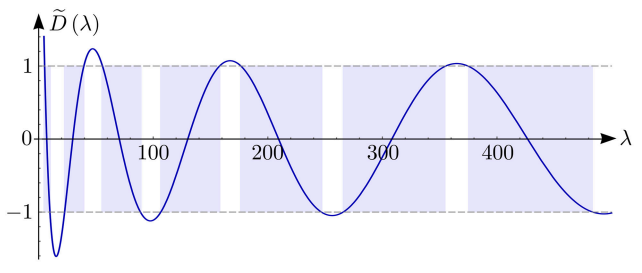

FIGURE 1 | Plot of the approximate function $\widetilde{D}(\lambda)$ for the Kronig-Penney model from Example 1.

corresponding to $\lambda = \lambda_0$, then the series

$$u_{1,j}(x) = u_{0,j}(x)\sum_{k=0}^{\infty}(\lambda - \lambda_0)^k\,\widetilde{X}_j^{(2k)}(x),$$

$$u_{2,j}(x) = u_{0,j}(x)\sum_{k=0}^{\infty}(\lambda - \lambda_0)^k\,X_j^{(2k+1)}(x)$$

satisfy equation (21) in the interval e_j $(j = 0, \cdots, N)$.

5. NUMERICAL EXAMPLES

In this section we employ the SPPS approach for the calculation of the band edges of the spectral bands of periodic Schrödinger operators with point interactions. For this aim we use the approximate version $\widetilde{D}(\lambda)$ of the function $D(\lambda)$ given by (31), and fix $N = 200$ as the number of terms in the approximate solutions $\widetilde{u}_{1,j}$ and $\widetilde{u}_{2,j}$. This implies calculating finite sets of formal powers $\left\{\widetilde{X}_j^{(k)}\right\}_{k=0}^{2N}$ and $\left\{X_j^{(k)}\right\}_{k=0}^{2N+1}$ according to recursive integration procedure (30). We employ of Wolfram Mathematica for the numerical study of the spectra of the examples considered in this section. For accurately handling the upper formal powers, even the double-precision floating-point format is not enough, nonetheless Wolfram Mathematica provides the instruction `SetPrecision[]` for increase the precision of the numbers. In this work we fix the precision of numerical results up to 100 decimal places. For the numerical implementation of our approach we distinguish two main parts, namely, calculating the formal powers, and searching for the zeros of the equation

$$\left|\widetilde{D}\left(\lambda_{\text{edge}}\right)\right| = 1$$

that define the band edges.

For calculating the formal powers, the integrands are numerically handled by an array of their values at a discrete set $\Omega_j \subset \overline{e_j}$ of $M + 1$ points. These values are interpolated by cubic splines with the instruction `Interpolation[]`, and then integrated by the instruction `Integrate[]`. Here we have segmented each $\overline{e_j}$ into $M = 2,000$ parts. Once formal powers are computed, approximate monodromy matrices $\widetilde{\mathbf{M}}_{j,j+1}(\lambda)$ are determined from the functions $\widetilde{\phi}_{1,j}(x)$ and $\widetilde{\phi}_{2,j}(x)$, which were calculated at the points of Ω_j. In turn these matrices lead to the approximate transmission matrix $\widetilde{\mathbf{T}}$ that defines the function $\widetilde{D}(\lambda)$ according to (31). Calculating the band edges reduces to calculating the polynomial roots of $\widetilde{D}(\lambda) \pm 1 = 0$. We use the instruction `FindRoot[]` to search for numerical solutions of the polynomial equations near the real axis of the complex λ-plane. We prescribe a small tolerance $\varepsilon > 0$ such that if the imaginary part of a root λ_j satisfies $\left|\Im\lambda_j\right| \leq \varepsilon$ then its real part can be considered as an approximate band edge, that is, $\lambda_{\text{edge}} = \Re\lambda_j$.

Example 1 (Kronig-Penney model)**.** Let us consider the Kronig-Penney model with the singular potential specified by (26). It was shown that transmission matrix in this case reads $\mathbf{T}(\lambda) =$

$\mathbf{M}_{1,2}(\lambda)\,\mathbf{A}_\alpha\mathbf{M}_{0,1}(\lambda)$, where matrix $\mathbf{A}_\alpha$ is defined in (27). For showing the accuracy of the SPPS approach, in this example we compare the zeros from of the approximate equations $\widetilde{D}(\lambda)\pm 1 = 0$ and those obtained from the exact Kronig-Penney relation (28), where we take $\alpha = 10$ and $\ell = 1$, see **Figure 1**. In **Table 1** we can see that the results coincide in at least eight decimal places in the least accurate results, and up to fourteen decimal places in the most accurate result. The loss in accuracy is due to the fact that truncated power series with center at $\lambda = 0$ depart from exact solutions as $|\lambda|$ increases. The accuracy of the results can be improved by either increasing the number of subdivisions of the intervals $\overline{e_j}$, by increasing the number N of terms of the truncated series, or by means of the shifting of the spectral parameter, in which power series are expanded about another center $\lambda_0 \neq 0$, as was explained above.

Example 2 (Potential without point interactions)**.** Suppose that operator S_q has a potential q consisting on only the regular part q_0 defined by

$$q_0(x) = -2 - \operatorname{sech}(x-2), \quad 0 \le x < 4, \tag{32a}$$

$$q_0(x+4) = q_0(x), \quad \forall x \in \mathbb{R}. \tag{32b}$$

It follows that $n = 0$, $\ell = 4$, and $\mathcal{Y}_0 = \emptyset$. Operator S_{q_0} defines an unbounded operator $\mathcal{H}_{q_0}$ in $L^2(\mathbb{R})$ with domain $H^2(\mathbb{R})$. The transmission matrix is given by $\mathbf{T} = \mathbf{M}_{0,1}$, where the monodromy matrix

$$\mathbf{M}_{0,1}(\lambda) = \begin{pmatrix} \phi_1(\ell;\lambda) & \phi_2(\ell;\lambda) \\ (\phi_1)'_x(\ell;\lambda) & (\phi_2)'_x(\ell;\lambda) \end{pmatrix}$$

is defined from a pair of solutions ϕ_1, ϕ_2 of the equation $S_{q_0}u = \lambda u$, $0 < x < \ell$, satisfying the Cauchy conditions $\phi_1(0;\lambda) = 1$, $\phi_1'(0;\lambda) = 0$, $\phi_2(0;\lambda) = 0$, $\phi_2'(0;\lambda) = 1$. In this example the function $D(\lambda) = \frac{1}{2}\left(\phi_1(\ell;\lambda) + (\phi_2)'_x(\ell;\lambda)\right)$ is approximated by the SPPS approach described in subsection 4.3. In **Figure 2** we can see the plot of the approximate function $\widetilde{D}(\lambda)$ and its intersections with the horizontal lines ± 1 that define the spectral bands $[a_j, b_j]$. In **Table 2** we observe some spectral bands of $\mathcal{H}_{q_0}$, whose edges were calculated from the zeros of the equations $\widetilde{D}(\lambda) \pm 1 = 0$. The fourth and fifth columns of the table show the widths of the bands and the gaps, respectively. We can see a monotonically increasing of the band widths, while the gaps monotonically decrease. Such a behavior is a characteristic of smooth periodic potentials (see, e.g., [31]) The considered potential q_0 is smooth except at a countable set of points of the form $x_k = k\ell$, $k \in \mathbb{Z}$, nonetheless the potential is continuous at these points.

Example 3 (Potential including δ-interactions)**.** Let the potential q of Schrödinger operator S_q be a π-periodic function defined by

$$q(x) = q_0 + \sum_{n\in\mathbb{Z}} 2\delta\left(x + \left(n + \frac{1}{2}\right)\pi\right),$$

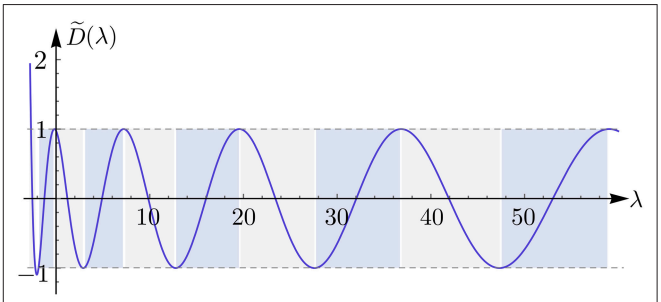

FIGURE 2 | Plot of the approximate function $\widetilde{D}(\lambda)$ from Example 2.

TABLE 2 | Some spectral bands $[a_j, b_j]$ of the Hamiltonian $\mathcal{H}_{q_0}$ from Example 2.

j	a_j	b_j	$b_j - a_j$	$a_j - b_{j-1}$
1	−2.67428666671436	−2.21034342939206	0.463943	–
2	−1.86953451704338	−0.18788534501576	1.68165	0.340809
3	−0.16355607594023	2.89703477791651	3.06059	0.0243293
4	2.91041104450921	7.21694695958455	4.30654	0.0133763
5	7.22365825701727	12.76922201025541	5.54556	0.0067113
6	12.77350452947204	19.55493528380191	6.78143	0.00428252
7	19.55787702778062	27.57420128901233	8.01632	0.00294174
8	27.57635166441515	36.82709282973720	9.25074	0.00215038
9	36.82873349589631	47.31364139486438	10.4849	0.00164067
10	47.31493463461126	59.03386368002606	11.7189	0.00129324

TABLE 1 | Some spectral bands of the Kronig-Penney model calculated from the SPPS approach and the exact expression (28).

	SPPS approach		**Exact Kronig-Penney expression**		**Absolute differences**	
j	a_j	b_j	a_j^*	b_j^*	$\lvert a_j - a_j^*\rvert$	$\lvert b_j - b_j^*\rvert$
1	5.21872875114394	9.86960440108947	5.21872875114393	9.86960440108935	1.06581×10^{-14}	1.19016×10^{-13}
2	22.66987264962470	39.47841760436475	22.66987264962356	39.47841760435743	1.14042×10^{-12}	7.31859×10^{-12}
3	55.70646200094253	88.82643960988765	55.70646200092423	88.82643960980421	1.82965×10^{-11}	8.34319×10^{-11}
4	106.63889490746644	157.91367041789846	106.63889490733228	157.91367041742975	1.34149×10^{-10}	4.68702×10^{-10}
5	176.52421330245437	246.74011002902202	176.52421330183057	246.74011002723395	6.23799×10^{-10}	1.78807×10^{-9}
6	265.79200348467112	355.30575844455604	265.79200348251038	355.30575843921678	2.16073×10^{-9}	5.33925×10^{-9}
7	374.62223620638347	483.61061566684185	374.62223620027810	483.61061565337854	6.10538×10^{-9}	1.34633×10^{-8}

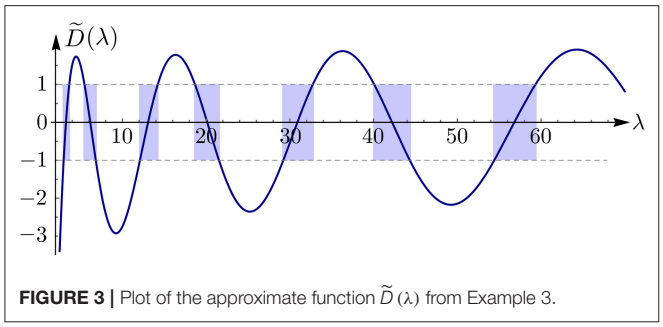

FIGURE 3 | Plot of the approximate function $\widetilde{D}(\lambda)$ from Example 3.

TABLE 3 | Some spectral bands $[a_j, b_j]$ of the Hamiltonian $\mathcal{H}_{q_0}$ from Example 3.

j	a_j	b_j	$b_j - a_j$	$a_j - b_{j-1}$
1	3.06183781347907	3.46162839690882	0.399791	–
2	5.69859494475109	6.52258314515798	0.823988	2.23697
3	12.41958132212809	13.72611107363096	1.30653	5.89699
4	19.18349016467425	20.94891270433824	1.76542	5.45738
5	29.80585404067745	31.98452624002360	2.17867	8.85694
6	40.84052913551672	43.46896744277874	2.62844	8.85600
7	55.26982482796178	58.31214991061162	3.04233	11.8009
8	70.47604145435538	73.95789867313669	3.48186	12.1639
9	88.77758666329101	92.67469008649469	3.89710	14.8197
10	108.09491317730821	112.42506663387381	4.33015	15.4202

where the regular potential is the piecewise continuous periodic function

$$q_0(x) = \begin{cases} \sin(2x) + 1, & 0 \le x < \pi/2, \\ -1, & \pi/2 \le x < \pi, \end{cases} \tag{33a}$$

$$q_0(x+\pi) = q_0(x), \quad \forall x \in \mathbb{R}. \tag{33b}$$

It follows that $n = 1$, $\ell = \pi$, and $\mathcal{Y}_0 = \{\pi/2\}$. The transmission matrix is given by $\mathbf{T}(\lambda) = \mathbf{M}_{1,2}(\lambda)\,\mathbf{A}_1\mathbf{M}_{0,1}(\lambda)$, where

$$\mathbf{A}_1 = \begin{pmatrix} 1 & 0 \\ 2 & 1 \end{pmatrix}.$$

The approximation of function $D(\lambda) = \frac{1}{2}(T_{11}(\lambda) + T_{22}(\lambda))$ obtained by the SPPS approach is plotted in **Figure 3**. In **Table 3** we observe some spectral bands of $\mathcal{H}_{q_0}$, whose edges were calculated from the zeros of the equations $\widetilde{D}(\lambda) \pm 1 = 0$. According to the fourth and fifth columns of the table we can see that both the band widths and gaps have a tendency to grow. Moreover, the band-to-gap ratio also has an exponential tendency to grow. This characteristic is shared by operators with singular potentials including point interactions (cf. [25]).

Example 4 (Potential including δ'-interactions)**.** Let us consider a periodic potential q involving δ'-interactions

$$q(x) = q_0 + \sum_{n\in\mathbb{Z}} \left(\delta'\left(x+n+\tfrac{1}{4}\right) + 2\delta'\left(x+n+\tfrac{1}{2}\right)\right),$$

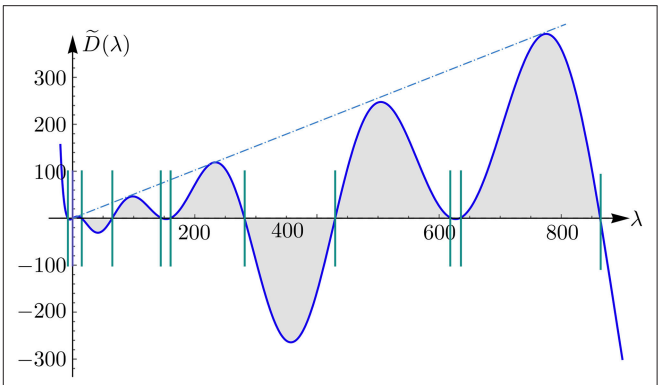

FIGURE 4 | Plot of the approximate function $\widetilde{D}(\lambda)$ from Example 4.

where the regular potential is defined by

$$q_0(x) = 4x - 2, \quad q_0(x+1) = q_0(x), \quad \forall x \in \mathbb{R}. \tag{34}$$

In this example $n = 2$, $\ell = 1$, and $\mathcal{Y}_0 = \left\{\frac{1}{4}, \frac{1}{2}\right\}$. The transmission matrix is given by

$$\mathbf{T}(\lambda) = \mathbf{M}_{2,3}(\lambda)\,\mathbf{A}_2\mathbf{M}_{1,2}(\lambda)\,\mathbf{A}_1\mathbf{M}_{0,1}(\lambda), \tag{35}$$

where

$$\mathbf{A}_1 = \begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix}, \quad \mathbf{A}_2 = \begin{pmatrix} 1 & -2 \\ 0 & 1 \end{pmatrix}.$$

The approximate function $\widetilde{D}(\lambda)$ obtained from the SPPS approach is plotted in **Figure 4**. In this case the spectral bands are indicated by thin vertical strips in the plot. In **Table 4** we observe some spectral bands of $\mathcal{H}_{q_0}$ calculated from the zeros of the equations $\widetilde{D}(\lambda) \pm 1 = 0$. The table shows a narrowness of the bands compared with the large gaps, which can be understood on the fact that at the high values of λ the unit cells of the periodic problem get decoupled since δ'-interaction approximates to Neumann conditions [25, 26]. We also observe that the peaks of the plot of $\widetilde{D}$ are dominated by a straight line with positive slope, which accounts for the increasing gaps of the spectrum. The considered problem has spectral properties that resemble those of Wannier-Stark ladders for a periodic array of δ'-scatterers [26]. These observations agree with the spectra of systems with periodically distributed δ'-distributions (see, e.g., [22, 27, 28]).

Example 5 (Potential including both δ- and δ'-interactions)**.** In this example we consider the following periodic potential

$$q(x) = q_0 + \sum_{n\in\mathbb{Z}} \left(2\delta\left(x+n+\tfrac{1}{4}\right) - 2\delta'\left(x+n+\tfrac{3}{4}\right)\right),$$

which involves both δ- and δ'-interactions, where the regular potential is given by

$$q_0(x) = 10\left(x - \tfrac{1}{2}\right)^2, \quad q_0(x+1) = q_0(x), \quad \forall x \in \mathbb{R}.$$

TABLE 4 | Some spectral bands $[a_j, b_j]$ of the Hamiltonian $\mathcal{H}_{q_0}$ from Example 4.

j	a_j	b_j	$b_j - a_j$	$a_j - b_{j-1}$
1	−7.85411657153512	−6.83369602987881	1.02042	—
2	−0.65046048277948	1.84587555882338	2.49634	6.18324
3	11.65425503800808	13.43273085127024	1.77848	9.80838
4	68.26969354771300	69.03634328596869	0.76665	54.8369
5	144.85052700115227	148.79531015416193	3.94478	75.8142
6	157.67353066071464	161.42975111317477	3.75622	8.87822
7	273.31957684722038	273.70125145939630	0.38167	111.8898
8	439.51292832002877	439.81704937865748	0.30412	165.8116
9	618.73286597182914	622.54765426193728	3.81479	178.9158

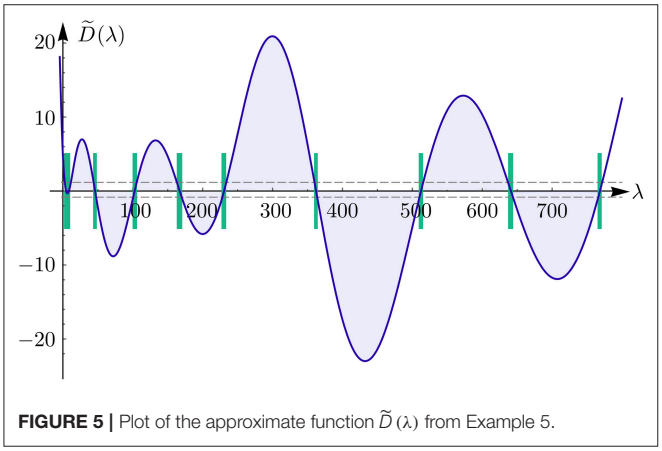

FIGURE 5 | Plot of the approximate function $\widetilde{D}(\lambda)$ from Example 5.

TABLE 5 | Some spectral bands $[a_j, b_j]$ of the Hamiltonian $\mathcal{H}_{q_0}$ from Example 5.

j	a_j	b_j	$b_j - a_j$	$a_j - b_{j-1}$
1	2.86762223529348	10.23246965803260	7.36485	—
2	45.56882948698923	48.61942765089296	3.05059	35.3364
3	101.27707819595177	106.08760865097772	4.81053	52.6577
4	163.54551092639027	170.36688233214974	6.82137	57.4579
5	225.66146649230063	231.02984943621416	5.36838	55.2946
6	361.63534945045842	364.93962223189151	3.30427	130.606
7	512.49899820086693	517.49353325243941	4.99454	147.559
8	637.30399761249782	644.20426504160877	6.90027	119.810
9	761.93050746223082	767.18997844883585	5.25947	117.726

TABLE 6 | Some spectral bands $[a_j, b_j]$ of the perturbed Hamiltonian $\mathcal{H}_{q_0+q_1}$ from Example 2.

j	$\tilde{a}_j = a_j + m^{\infty}_{q_1}$	$\tilde{b}_j = b_j + M^{\infty}_{q_1}$	$\tilde{b}_j - \tilde{a}_j$	$\tilde{a}_j - \tilde{b}_{j-1}$
1	−3.67428666671436	−1.21034342939206	2.46394	—
2	−2.86953451704338	0.81211465498424	3.68165	−1.65919
3	−1.16355607594023	3.89703477791651	5.06059	−1.97567
4	1.91041104450921	8.21694695958455	6.30654	−1.98662
5	6.22365825701727	13.76922201025541	7.54556	−1.99329
6	11.77350452947204	20.55493528380191	8.78143	−1.99572
7	18.55787702778062	28.57420128901233	10.0163	−1.99706
8	26.57635166441515	37.82709282973720	11.2507	−1.99785
9	35.82873349589631	48.31364139486438	12.4849	−1.99836
10	46.31493463461126	60.03386368002606	13.7189	−1.99871

In this case $n = 2$, $\ell = 1$, $\mathcal{Y}_0 = \left\{\frac{1}{4}, \frac{3}{4}\right\}$, and the transmission matrix is given by expression (35), where the matrices

$$\mathbf{A}_1 = \begin{pmatrix} 1 & 0 \\ 2 & 1 \end{pmatrix}, \quad \mathbf{A}_2 = \begin{pmatrix} 1 & 2 \\ 0 & 1 \end{pmatrix}.$$

On applying the SPPS approach we calculate the approximate function $\widetilde{D}(\lambda)$, which is shown in **Figure 5**. From the zeros of the equations $\widetilde{D}(\lambda) \pm 1 = 0$ we obtain the spectral bands of $\mathcal{H}_{q_0}$, which are shown in **Table 5**. The spectrum of this operator shares common characteristics with the previous spectra, for instance, the large gap-to-band ratio due to the presence of δ- and δ'-interactions.

Previous examples show the applicability of the SPPS method in the numerical determination of the spectral bands of periodic Schrödinger operators with point interactions. For numerically simulating the influence of a slowly oscillating at infinity potential q_1 on the gaps of the essential spectrum of the operators it is necessary to determine the numbers $m^{\infty}_{q_1}$ and $M^{\infty}_{q_1}$, and employ formula (19) for calculating the essential spectrum of the perturbed operator.

Example 6 (Perturbed periodic potential)**.** Let $q_1(x) = A \sin |x|^{\varepsilon}$, $\varepsilon \in (0, 1)$, $A > 0$, $x \in \mathbb{R}$. Since $q_1 \in \mathrm{SO}(\mathbb{R})$, it is easy to see that for every sequence $\mathbb{R} \ni h_m \to \infty$ the limit q_1^h is a real constant. The limiting values satisfy $\left|q_1^h\right| \leq A$ for every real sequence $h = \{h_m\}$, hence, $m^{\infty}_{q_1} = -A$ and $M^{\infty}_{q_1} = A$.

Let us consider the previous Example 2 and suppose that its regular potential q_0 defined in (32) is perturbed by the potential $q_1 \in \mathrm{SO}(\mathbb{R})$ with $A = 1$. In **Table 6** we observe the influence of this slowly oscillating function on the spectrum of the unperturbed operator $\mathcal{H}_{q_0}$. We observe the broadening of the bands and their corresponding overlapping when the gaps are negative. Since the gaps of the unperturbed problems are monotonically decreasing all the bands will overlap producing a continuous spectrum

$$\mathrm{sp}_{\mathrm{ess}}\mathcal{H}_{q_0+q_1} = \left[a_1 + m^{\infty}_{q_1}, +\infty\right) = [-3.67428666671436, +\infty).$$

Now, let us consider the previous Example 3, and suppose that its regular potential q_0 defined in (33) is perturbed by a more intense perturbation $q_1 \in \mathrm{SO}(\mathbb{R})$ with $A = 6$. The bands of the resulting perturbed operator $\mathcal{H}_{q_0+q_1}$ are shown in **Table 7**. In this case the first seven bands of the spectrum overlap, yielding the merged band

$$\left[a_1 + m^{\infty}_{q_1}, b_7 + M^{\infty}_{q_1}\right] = [-2.93816218652093, 64.31214991061162] \subset \mathrm{sp}_{\mathrm{ess}}\mathcal{H}_{q_0+q_1}.$$

TABLE 7 | Some spectral bands $[a_j, b_j]$ of the perturbed Hamiltonian $\mathcal{H}_{q_0+q_1}$ from Example 3.

j	$\tilde{a}_j = a_j + m^{\infty}_{q_1}$	$\tilde{b}_j = b_j + M^{\infty}_{q_1}$	$\tilde{b}_j - \tilde{a}_j$	$\tilde{a}_j - \tilde{b}_{j-1}$
1	−2.93816218652093	9.46162839690882	12.399791	—
2	−0.30140505524891	12.52258314515798	12.823988	−9.76303
3	6.41958132212809	19.72611107363096	13.30653	−6.10299
4	13.18349016467425	26.94891270433824	13.76542	−6.54262
5	23.80585404067745	37.98452624002360	14.17867	−3.14306
6	34.84052913551672	49.46896744277874	14.62844	−3.14399
7	49.26982482796178	64.31214991061162	15.04233	−0.19914
8	64.47604145435538	79.95789867313669	15.48186	0.163892
9	82.77758666329101	98.67469008649469	15.89710	2.819690
10	102.09491317730821	118.42506663387381	16.33015	3.420221

TABLE 8 | Some spectral bands $[a_j, b_j]$ of the perturbed Hamiltonian $\mathcal{H}_{q_0+q_1}$ from Example 4.

j	$\tilde{a}_j = a_j + m^{\infty}_{q_1}$	$\tilde{b}_j = b_j + M^{\infty}_{q_1}$	$\tilde{b}_j - \tilde{a}_j$	$\tilde{a}_j - \tilde{b}_{j-1}$
1	−10.85411657153512	−3.83369602987881	7.02042	—
2	−3.65046048277948	4.84587555882338	8.49634	0.18323
3	8.65425503800808	16.43273085127024	7.77848	3.80838
4	65.26969354771300	72.03634328596869	6.76665	48.8369
5	141.85052700115227	151.79531015416193	9.94478	69.8142
6	154.67353066071464	164.42975111317477	9.75622	2.87822
7	270.31957684722038	276.70125145939630	6.38167	105.8899
8	436.51292832002877	442.81704937865748	6.30412	159.8119
9	615.73286597182914	625.54765426193728	9.81479	172.9158

From the eighth band, the gaps of the spectrum are open. Hence, in order to close more gaps, it is necessary to increase the intensity of the perturbation.

Finally, on considering the potential (34) from Example 4 and the perturbation $q_1 \in \mathrm{SO}(\mathbb{R})$ with $A = 3$ we obtain the spectral bands shown in **Table 8**. In this case, though the bands get broader, none of them overlap with the given perturbation.

6. CONCLUSIONS

In this work we have approached one-dimensional Schrödinger operators with point interactions from their corresponding self-adjoint extensions. On assuming that the point interactions are supported on an infinite countable set with a periodic structure we were able to employ the limit operators method for analyzing their essential spectra. If the regular potentials are periodic the Floquet-Bloch theory leads to a formula defining the band-gap spectra of the periodic operators, which is given in terms of a function $D(\lambda)$. This function is obtained from the monodromy matrices specified at the points where the singular potential is supported. In this work the function $D(\lambda)$ is determined by the SPPS method, which allows to consider arbitrary regular potentials q_0 satisfying certain smoothness conditions, and to derive numerical methods for calculating the band edges of spectra of periodic problems involving point interactions.

We also considered the case when periodic problems are perturbed by slowly oscillating at infinity terms, which can model impurities in the crystals. The perturbed problems are also approached by the limit operators method, which gives a neat formula for their essential spectra. The spectral analysis of perturbed periodic problems relies on a pair of numbers $m^{\infty}_{q_1}$ and $M^{\infty}_{q_1}$ that depend on the perturbation $q_1 \in \mathrm{SO}(\mathbb{R})$ specified in the problem. These numbers, in general, lead to the broadening (narrowing) of the bands (gaps), which may change significantly the spectra of the operators. The SPPS approach together with the determination of the numbers $m^{\infty}_{q_1}$, $M^{\infty}_{q_1}$ give a simpler way for determining the spectra of perturbed periodic problems.

The applicability of the SPPS method and the limit operators method is shown by the numerical examples considered in this work that involved δ- and δ'-interactions as well as a periodic regular potential q_0. The accuracy of the results relies on the uniform convergence of power series of the spectral parameter that define the solutions of the involved Schrödinger equations, so that an increasingly number N of terms in the truncated series will reduce the associated errors in the numerical values. Finally, the theory developed in this work can be used for analyzing photonic crystals and electromagnetic waveguides with periodic refractive profiles, as well as quantum problems involving periodic potentials.

DATA AVAILABILITY

All datasets generated and analyzed for this study are included in the manuscript and the supplementary files.

AUTHOR CONTRIBUTIONS

VR conceived the idea of the paper and developed the theoretical formalism. VB-F performed the analytic calculations, designed the examples, and analyzed the numerical data. VR, VB-F, and LO contributed to the final version of the manuscript.

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Some Remarks on 1D Schrödinger Operators With Localized Magnetic and Electric Potentials

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One-dimensional Schrödinger operators with singular perturbed magnetic and electric potentials are considered. We study the strong resolvent convergence of two families of the operators with potentials shrinking to a point. Localized δ-like magnetic fields are combined with δ'-like perturbations of the electric potentials as well as localized rank-two perturbations. The limit results obtained heavily depend on zero-energy resonances of the electric potentials. In particular, the approximation for a wide class of point interactions in one dimension is obtained.

Keywords: 1D Schrödinger operator, magnetic potential, zero-energy resonance, half-bound state, short range interaction, point interaction, δ-potential, δ'-potential

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1. INTRODUCTION

The present paper is concerned with the convergence of families of singularly perturbed one-dimensional magnetic Schrödinger operators. Our motivation of the study on this convergence comes from an application to the scattering of quantum particles by sharply localized potentials and finite rank perturbations. The main purpose is to construct solvable models in terms of the point interactions describing with admissible fidelity the real quantum interactions. The Schrödinger operators with potentials that are distributions supported on discrete sets (such potentials are usually termed point interactions) have attracted considerable attention since the 1980s. It is an extensive subject with a large literature (see [1, 2], and the references given therein).

It is well-known that all nontrivial point interactions at a point x can be described by the coupling conditions

$$\begin{pmatrix} \psi(x+0) \\ \psi'(x+0) \end{pmatrix} = e^{i\varphi} \begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix} \begin{pmatrix} \psi(x-0) \\ \psi'(x-0) \end{pmatrix}, \tag{1.1}$$

where $\varphi \in [-\frac{\pi}{2}, \frac{\pi}{2}]$, $c_{kl} \in \mathbb{R}$, and $c_{11}c_{22} - c_{12}c_{21} = 1$ (see, e.g., [3, 4]). The nontriviality of point interactions means that the associated self-adjoint operator cannot be presented as a direct sum of two operators acting in $L_2(-\infty, 0)$ and $L_2(0, \infty)$. For the quantum systems described by the Schrödinger operators with regular potentials localized in a neighborhood of x one can often assign the Schrödinger operators with the point interactions (1.1) so that the corresponding zero-range models govern the quantum dynamics of the true interactions with adequate accuracy, especially for the low-energy particles. In this context, the inverse problem is also of interest. The important question is how to approximate a given point interaction by Schrödinger operators with localized regular potentials or finite-rank perturbations.

We study the families of the Schrödinger operators that can be partially viewed as regularizations of the pseudo-Hamiltonians

$$\begin{gathered}\left(i\frac{d}{dx}+a\delta(x)\right)^2+b\delta'(x)+c\delta(x),\\ \left(i\frac{d}{dx}+a\delta(x)\right)^2+b\big(\langle\delta'(x),\,\cdot\,\rangle\,\delta(x)+\langle\delta(x),\,\cdot\,\rangle\,\delta'(x)\big)+c\delta(x),\end{gathered}\tag{1.2}$$

where δ is Dirac's delta function. We note that $\delta'(x)y = y(0)\delta'(x) - y'(0)\delta(x)$ for continuously differentiable functions y at the origin. Thus we may formally regard the δ' potential as rank-two perturbation $\delta'(x)y = \langle\delta(x), y\rangle\,\delta'(x) + \langle\delta'(x), y\rangle\,\delta(x)$. However, both the heuristic operators have generally no mathematical meaning. So it is not surprising that different regularizations of the distributions in (1.2) lead to different self-adjoint operators in the limit. Therefore, the pseudo-Hamiltonians (1.2) can be regarded as a symbolic notation only for a wide variety of quantum systems with quite different properties depending on the shape of the short-range potentials.

Recently a class of the Schrödinger operators with piecewise constant δ'-potentials were studied by Zolotaryuk [5–8]; the resonances in the transmission probability for the scattering problem were established. As was shown in Golovaty et al. [9], Golovaty and Hryniv [10, 11], and Man'ko [12] these resonances deal with the existence of zero-energy resonances and the half-bound states for singular localized potentials. The zero-energy resonances have a profound effect on the limiting behavior of the Schrödinger operators with δ'-potentials. Such operators also arose in connection with the approximation of smooth planar quantum waveguides by quantum graph [13–15]; a similar resonance phenomenon was obtained. The reader also interested in the literature on other aspects of δ'-potentials and δ'-interactions as well as approximations of point interactions by local and non-local perturbations is referred to Albeverio and Nizhnik [16], Albeverio et al. [17, 18], Exner and Manko [19], Gadella et al. [20–22].

It is known that one dimensional Schrödinger operators

$$H(b)=\left(i\frac{d}{dx}+b(x)\right)^2+V(x)$$

with continuous magnetic potentials are not especially interesting, because any continuous field b is equivalent under a smooth gauge transformation to 0. This means that the operator $H(b)$ with a continuous gauge field is unitarily equivalent to the Schrödinger operator $H(0) = -\frac{d^2}{dx^2} + V(x)$ without a magnetic field. The authors of Coutinho et al. [23] have even asserted that the phase parameter φ in conditions (1.1) is redundant and it produces no interesting effect. They have stated that if the time-reversal invariance is imposed, the number of the parameters that specify the interactions (1.1) can be reduced to three.

For the case of singular magnetic potentials, however, there are certain nontrivial examples [24], pointing out that this case is more subtle. Albeverio et al. [24] have shown that the phase parameter is not redundant if non-stationary problems are concerned. The phase parameter can be interpreted as the amplitude of a singular gauge field. As stated in Kurasov [25] a nonzero phase φ in the coupling conditions (1.1) may appear if and only if the singular gauge field is present. However, it is noteworthy that the factor $e^{i\varphi}$ also appeared in the solvable model for the Schrödinger operators without a magnetic field that is perturbed by a rank-two operator [26]. We also want to note that Theorem 2 in the present paper gives an example of an exactly solvable model in which the magnetic field has an effect on all coefficients c_{kl} in (1.1), not only on factor $e^{i\varphi}$.

Another reason to study the 1-D Schrödinger operators with magnetic fields comes from the quantum graph theory which is a useful tool in modeling numerous physical phenomena. One of the fundamental questions of this theory consists of justifying the possibility of approximating dynamics of a quantum particle confined to real-world mesoscopic waveguides of small width d by its dynamics on the graph obtained in the limit as d vanishes. In Exner et al. [27], the authors demonstrated that any self-adjoint coupling in a quantum graph vertex can be approximated by a family of magnetic Schrödinger operators on a tubular network built over the graph.

The magnetic Schrödinger operators and the Dirac Hamiltonians with Aharonov-Bohm fields have been discussed from various aspects by many authors. We confine ourself to a brief overview of the most relevant papers. For the mathematical foundation of the magnetic Schrödinger operators we refer the reader to the paper of Avron et al. [28]. In two dimension, the norm resolvent convergence of the Schrödinger operators

$$\mathcal{H}_\varepsilon=\big(i\nabla+\varepsilon^{-1}A(x/\varepsilon)\big)^2+\varepsilon^{-2}V(x/\varepsilon)$$

with singularly scaled magnetic and electric potentials was studied by Tamura [29]. The magnetic potential had the δ-like field $\varepsilon^{-2}b(x/\varepsilon) = \varepsilon^{-1}\nabla\times A(x/\varepsilon)$, and b and V were smooth vector functions in $\mathbb{R}^2$ of compact support. The limit operator strongly depends on the total flux of magnetic field and on the resonance space at zero energy. The scattering by a magnetic field with small support and the convergence to the scattering amplitude by δ magnetic field were studied in Tamura [30]. In Tamura [31], the case of relativistic particles moving in the Aharonov-Bohm magnetic field with a δ-like singularity was considered. The author approximated the point–like field by smooth ones and found the limit self-adjoint operators uniquely specified by physically and mathematically reasonable boundary conditions at the origin.

The present paper can be viewed as a natural continuation of our previous works [26, 32–34], in which the case without of a magnetic field was treated.

2. STATEMENT OF PROBLEM AND MAIN RESULTS

Let us consider the Schrödinger operator

$$H_0=-\frac{d^2}{dx^2}+V_0$$

in $L_2(\mathbb{R})$, where potential V_0 is real-valued, measurable and locally bounded. We also assume that V_0 is bounded from below in $\mathbb{R}$. We turn now to our primary task of studying the limit behavior of two families of operators in $L_2(\mathbb{R})$, which can be treated as perturbations of H_0.

2.1. Hamiltonians With Localized Potentials

First we consider the self-adjoint operators

$$\mathcal{H}_{\varepsilon\nu} = \Big(i\,\frac{d}{dx} + \frac{1}{\varepsilon}\,A\Big(\frac{x}{\varepsilon}\Big)\Big)^2 + V_0(x) + \frac{\alpha}{\varepsilon^2}\,V\Big(\frac{x}{\varepsilon}\Big) + \frac{1}{\nu}\,U\Big(\frac{x}{\nu}\Big), \quad (2.1)$$

where ε and ν are small positive parameters, and α is a real coupling constant. Let A, V, and U be real-valued, measurable, and bounded functions of compact support. Suppose furthermore that $A \in \mathcal{AC}(\mathbb{R})$. The domain of $\mathcal{H}_{\varepsilon\nu}$ coincides with $\operatorname{dom} H_0$, because the perturbation has a compact support. Note that we consciously equipped potential V only with a coupling constant. As we will see later, the limit behavior of $\mathcal{H}_{\varepsilon\nu}$ crucially depends on α.

The potentials $\alpha\varepsilon^{-2}V(\varepsilon^{-1}x) + \nu^{-1}U(\nu^{-1}x)$ converge, as ε and ν go to zero, to a distribution having the form $b_1\delta'(x) + b_0\delta(x)$, if V has a zero-mean value, and they diverge otherwise. Hence parameter ε describes the rate of shrinking for the δ'-like potential (as well as the magnetic potential), while ν is the rate of shrinking for the δ-like potential. The sequence $\varepsilon^{-1}A(\varepsilon^{-1}x)$ converges to $\mu\delta(x)$ as $\varepsilon \to 0$ in the sense of distributions, where

$$\mu = \int_{\mathbb{R}} A(x)\,dx. \quad (2.2)$$

In the partial cases, operators $\mathcal{H}_{\varepsilon\nu}$ can be regarded as a regularization of the first pseudo-Hamiltonian in (1.2).
Let us introduce some characteristics of the potentials V and U.

Definition 1. *We say that the Schrödinger operator $-\frac{d^2}{dx^2} + \alpha V$ in $L_2(\mathbb{R})$ possesses a* zero-energy resonance *if there exists a non trivial solution $v_\alpha : \mathbb{R} \to \mathbb{R}$ of the equation $-v'' + \alpha V v = 0$ that is bounded on the whole line. We call v_α the* half-bound state *of αV.*

We will simply say that the potential αV is *resonant* and it possesses a half-bound state v_α. Let us denote by $\mathcal{R}(V)$ the set of all coupling constants α for which the potential αV is resonant, and introduce the mapping $\theta : \mathcal{R}(V) \to \mathbb{R}$ defined by

$$\theta(\alpha) = \frac{v_\alpha^+}{v_\alpha^-}, \quad (2.3)$$

where $v_\alpha^- = \lim\limits_{x\to-\infty} v_\alpha(x)$ and $v_\alpha^+ = \lim\limits_{x\to+\infty} v_\alpha(x)$. Let $\Lambda = [0, +\infty]$ be the set containing the point $+\infty$.

We also define the mapping $\gamma : \mathcal{R}(V) \times \Lambda \to \mathbb{R}$ as follows:

$$\gamma(\alpha, 0) = \frac{v_\alpha^2(0)}{v_\alpha^-\,v_\alpha^+} \int_{\mathbb{R}} U\,dt, \quad (2.4)$$

$$\gamma(\alpha, \lambda) = \frac{1}{v_\alpha^-\,v_\alpha^+} \int_{\mathbb{R}} U(t)\,v_\alpha^2(\lambda t)\,dt \qquad \text{for } \lambda \in (0, +\infty), \quad (2.5)$$

$$\gamma(\alpha, +\infty) = \theta(\alpha)\int_{\mathbb{R}_+} U\,dt + \theta(\alpha)^{-1}\int_{\mathbb{R}_-} U\,dt. \quad (2.6)$$

We follow the notation used in Golovaty [33]. This mapping describes different kinds of the resonance interactions between the potentials αV and U in the limit. Both the mappings θ and γ are well defined as we will show below in Lemma 1.

Let us introduce the subspace $\mathcal{V}$ in $L_2(\mathbb{R})$ as follows. We say that h belongs to $\mathcal{V}$ if there exist two functions h_- and h_+ belonging to $\operatorname{dom} H_0$ such that $h(x) = h_-(x)$ for $x < 0$ and $h(x) = h_+(x)$ for $x > 0$.

Theorem 1. *Suppose that a sequence $\{\nu_\varepsilon\}_{\varepsilon>0}$ of positive numbers is such that $\nu_\varepsilon \to 0$ and ratio $\nu_\varepsilon/\varepsilon$ tends to $\lambda \in \Lambda$ as $\varepsilon \to 0$, i.e., this ratio has a finite or infinite limit. If $\alpha \in \mathcal{R}(V)$, then family of operators $\mathcal{H}_{\varepsilon\nu_\varepsilon}$ converges in the strong resolvent sense as $\varepsilon \to 0$ to the operator $\mathcal{H} = \mathcal{H}(\alpha, \lambda)$ defined by $\mathcal{H}\phi = -\phi'' + V_0\phi$ on functions ϕ in $\mathcal{V}$ subject to the conditions*

$$\begin{pmatrix}\phi(+0)\\ \phi'(+0)\end{pmatrix} = e^{i\mu}\begin{pmatrix}\theta(\alpha) & 0\\ \gamma(\alpha,\lambda) & \theta(\alpha)^{-1}\end{pmatrix}\begin{pmatrix}\phi(-0)\\ \phi'(-0)\end{pmatrix}. \quad (2.7)$$

By analogy with the results in Golovaty [33], if potential αV is not resonant, the limit operator is the direct sum of two Dirichlet operators acting in $L_2(-\infty, 0)$ and $L_2(0, +\infty)$; that is, coupling conditions (2.7) must be substituted by the Dirichlet condition $\phi(0) = 0$.

It is worth noting that explicit relations (2.3)-(2.6) between the matrix entries $\theta(\alpha)$, $\gamma(\alpha, \lambda)$ and potentials V and U make it possible to carry out a quantitative analysis of this quantum system, e.g., to compute approximate values of the scattering data.

2.2. Hamiltonians With Localized Rank-Two Perturbations

We now turn our attention to another family of operators

$$\mathcal{T}_\varepsilon = \Big(i\,\frac{d}{dx} + \frac{1}{\varepsilon}\,A\Big(\frac{x}{\varepsilon}\Big)\Big)^2 + V_0(x) + \frac{1}{\varepsilon^3}\,F_\varepsilon + \frac{1}{\varepsilon}\,U\Big(\frac{x}{\varepsilon}\Big), \quad (2.8)$$

where $F_\varepsilon = F_\varepsilon(f_1, f_2)$ are rank-two operators having the form

$$\begin{aligned}(F_\varepsilon\phi)(x) &= \bar\beta\,\langle f_2(\varepsilon^{-1}\cdot), \phi\rangle\, f_1\Big(\frac{x}{\varepsilon}\Big) + \beta\,\langle f_1(\varepsilon^{-1}\cdot), \phi\rangle\, f_2\Big(\frac{x}{\varepsilon}\Big)\\ &= \int_{\mathbb{R}} \Big(\bar\beta f_1\Big(\frac{x}{\varepsilon}\Big)\bar f_2\Big(\frac{s}{\varepsilon}\Big) + \beta\bar f_1\Big(\frac{s}{\varepsilon}\Big) f_2\Big(\frac{x}{\varepsilon}\Big)\Big)\phi(s)\,ds. \quad (2.9)\end{aligned}$$

Here $\langle\cdot,\cdot\rangle$ is the inner scalar product $L_2(\mathbb{R})$. From now on, the norm in $L_2(\mathbb{R})$ will be denoted by $\|\cdot\|$. Operators $\mathcal{T}_\varepsilon$ can be viewed as a regularization of the second pseudo-Hamiltonian in (1.2). Assume that f_1, f_2 and q are measurable and bounded functions of compact support and β is a complex coupling constant. The potential q is real-valued.

Let us also consider rank-two perturbation of the free the Schrödinger operator

$$B = -\frac{d^2}{dx^2} + \bar\beta\,\langle h_2, \cdot\rangle\, h_1 + \beta\,\langle h_1, \cdot\rangle\, h_2, \quad \operatorname{dom} B = W_2^2(\mathbb{R}),$$

where h_1 and h_2 are functions of compact support.

Definition 2. *We say that operator B possesses a* zero-energy resonance *provided there exists a nontrivial solution of the equation*

$$-v'' + \bar{\beta}\,\langle h_2, v\rangle\, h_1 + \beta\,\langle h_1, v\rangle\, h_2 = 0 \tag{2.10}$$

that is bounded on the whole line. This solution is called a half-bound state *of B. We also say that B admits a* double zero-energy resonance, *if there exist two linearly independent half-bound states.*

We will denote by $\mathcal{R}(h_1, h_2)$ the set of all coupling constants β, for which operator B admits a double zero-energy resonance.

Let $h^{(-1)}$ and $h^{(-2)}$ be the first and second antiderivatives

$$h^{(-1)}(x) = \int_{-\infty}^{x} h(s)\,ds, \qquad h^{(-2)}(x) = \int_{-\infty}^{x} (x-s)h(s)\,ds$$

for functions of compact support. Note if h has zero mean, then $h^{(-1)}$ is also a function of compact support. Also, we set

$$a(x) = \int_{-\infty}^{x} A(t)\,dt. \tag{2.11}$$

Let us introduce notation

$$g_k = e^{-ia} f_k, \quad n_k = \|g_k^{(-1)}\|, \quad p = \langle {g_1}^{(-1)}, {g_2}^{(-1)}\rangle, \tag{2.12}$$

provided g_1 and g_2 are functions of zero mean values. Therefore n_k and p are well defined, since $g_k^{(-1)}$ are functions of compact support. Let

$$\omega_\beta = e^{i\arg(\beta^{-1}+p)} n_2 g_1^{(-2)} - n_1 g_2^{(-2)}.$$

Function ω_β is constant outside some compact set containing the supports of f_k. Of course $\omega_\beta(x) = 0$ for negative x with the large absolute value. Write

$$\varkappa = \lim_{x\to+\infty} \omega_\beta(x).$$

In the case of the double zero-energy resonance function ω_β is a half-bound state of B with $h_k = g_k$ (see Lemma 2 below). We also set

$$a_0 = \int_{\mathbb{R}} U\,dx, \qquad a_1 = \int_{\mathbb{R}} U\,\omega_\beta\,dx, \qquad a_2 = \int_{\mathbb{R}} U\,|\omega_\beta|^2\,dx.$$

Theorem 2. *Assume that f_1 and f_2 are linearly independent, $e^{-ia}f_1$ and $e^{-ia}f_2$ have zero means, and $\beta \in \mathcal{R}(e^{-ia}f_1, e^{-ia}f_2)$. Suppose also that $a_2 \neq \bar{\varkappa} a_1$. Then operator family $\mathcal{T}_\varepsilon$ converges as $\varepsilon \to 0$ in the strong resolvent sense to operator $\mathcal{T}$ defined by $\mathcal{T}\phi = -\phi'' + V_0\phi$ on functions ϕ in $\mathcal{V}$ subject to the conditions*

$$\begin{pmatrix}\phi(+0)\\ \phi'(+0)\end{pmatrix} = e^{i\left(\mu - \arg(a_2 - \overline{\varkappa} a_1)\right)} \begin{pmatrix} \dfrac{a_0|\varkappa|^2 - 2\mathrm{Re}(\overline{\varkappa} a_1) + a_2}{|a_2 - \overline{\varkappa} a_1|} & \dfrac{|\varkappa|^2}{|a_2 - \overline{\varkappa} a_1|} \\ \dfrac{a_0 a_2 - |a_1|^2}{|a_2 - \overline{\varkappa} a_1|} & \dfrac{a_2}{|a_2 - \overline{\varkappa} a_1|} \end{pmatrix} \begin{pmatrix}\phi(-0)\\ \phi'(-0)\end{pmatrix}. \tag{2.13}$$

Note in these conditions that parameters a_1, a_2 and $\varkappa$ depend nonlinearly on coupling constant β as well as functions f_1, f_2, a via ω_β; all elements of the matrix are real, since a_0 and a_2 are real number. The limit operator $\mathcal{T}$ is self-adjoint, because the determinant of matrix in (2.13) is equal to 1 [cf. (1.1)]. In fact,

$$\begin{aligned} &|a_2 - \overline{\varkappa} a_1|^{-2} \det \begin{pmatrix} a_0|\varkappa|^2 - 2\mathrm{Re}(\overline{\varkappa} a_1) + a_2 & |\varkappa|^2 \\ a_0 a_2 - |a_1|^2 & a_2 \end{pmatrix} \\ &= |a_2 - \overline{\varkappa} a_1|^{-2}\left(a_0 a_2|\varkappa|^2 - 2a_2\mathrm{Re}(\overline{\varkappa} a_1) + a_2^2 - a_0 a_2|\varkappa|^2 + |\varkappa|^2|a_1|^2\right) \\ &= |a_2 - \overline{\varkappa} a_1|^{-2}\left(a_2^2 - 2a_2\mathrm{Re}(\overline{\varkappa} a_1) + |\varkappa|^2|a_1|^2\right) \\ &= |a_2 - \overline{\varkappa} a_1|^{-2}\,|a_2 - \overline{\varkappa} a_1|^2 = 1. \end{aligned}$$

Though conditions (2.13) contain the full matrix, we can not assert that it is possible to approximate any point interaction (1.1) by operators $\mathcal{T}_\varepsilon$. For instance, such approximation does not exist for the point interactions (1.1) with matrices

$$\begin{pmatrix} c_{11} & 0 \\ c_{21} & c_{11}^{-1} \end{pmatrix},$$

where c_{11} is different from 1; if $\varkappa = 0$, then the matrix in (2.13) has the unit diagonal. Therefore, Theorems 1 and 2 are in some sense mutually complementary.

Remark also that for any pair of linearly independent functions f_1, f_2 satisfying the assumptions of the theorem there exists a wide class of potentials U for which condition $a_2 \neq \bar{\varkappa} a_1$ holds.

In view of Theorems 1 and 2 in Golovaty [26] we can expect that there exist at least six essentially different cases of the limiting behavior for $\mathcal{T}_\varepsilon$ as $\varepsilon \to 0$. However, in this paper we restrict ourselves to analyzing only the case that is described in Theorem 2. Just this case covers the widest class of point interactions in the limit.

3. ZERO-ENERGY RESONANCES AND HALF-BOUND STATES

We show first that the set $\mathcal{R}(V)$ of all resonance coupling constants for operator $-\frac{d^2}{dx^2} + \alpha V$ is not empty and furthermore it is rich enough for any function V of compact support.

Lemma 1. *(i) For each measurable function V of compact support, the resonant set $\mathcal{R}(V)$ is a countable subset of the real line with one or two accumulation points at infinity.*

(ii) For each $\alpha \in \mathcal{R}(V)$, the corresponding half-bound state v_α is unique up to a scalar factor. Moreover, both the limits

$$v_\alpha^- = \lim_{x\to-\infty} v_\alpha(x), \qquad v_\alpha^+ = \lim_{x\to+\infty} v_\alpha(x) \tag{3.1}$$

exist and are different from zero.

Proof: Without loss of generality we assume that $\mathrm{supp}\, V \subset \mathcal{I}$, where $\mathcal{I} = (-1, 1)$. Then operator $-\frac{d^2}{dx^2} + \alpha V$ possesses a half-bound state if and only if the problem

$$-v'' + \alpha V v = 0, \quad x \in \mathcal{I}, \qquad v'(-1) = 0, \quad v'(1) = 0 \tag{3.2}$$

has a non-trivial solution. In fact, a half-bound state ν_α is constant outside $\mathcal{I}$ as a bounded solution of equation $\nu'' = 0$ and hence $\nu'_\alpha(-1) = \nu'_\alpha(1) = 0$. From this we also deduce that there exist the limits (3.1). Obviously we have $\nu_\alpha^- = \nu_\alpha(-1)$ and $\nu_\alpha^+ = \nu_\alpha(1)$. In addition, both the values $\nu_\alpha(-1)$ and $\nu_\alpha(1)$ are different from zero in view of uniqueness for the Cauchy problem, because ν_α is a non-trivial solution.

Problem (3.2) can be regarded as a spectral problem with spectral parameter α. If V is a function of fixed sign, then (3.2) is a standard Sturm-Liouville problem and $\mathcal{R}(V)$ coincides with the spectrum of a self-adjoint operator in weighted Lebesgue spaces $L_2(V, \mathcal{I})$. Otherwise, we can interpret (3.2) as the eigenvalue problem with indefinite weight function V; the problem can be associated with a self-adjoint non-negative operator K in a Krein space [9, 32]. In both the cases the spectra of such operators are real and discrete with accumulation points at $-\infty$ or $+\infty$ only. Moreover all nonzero eigenvalues are simple; for the case of the Krein space, $\alpha = 0$ is generally semi-simple. The reader can also refers to Iohvidov et al. [35] for the details of the theory of self-adjoint operators in Krein spaces. It follows from the simplicity of spectra that half-bound state ν_α is unique up to a scalar factor. □

The set $\mathcal{R}(h_1, h_2)$ of coupling constants, for which the operator B possesses the double zero-range resonance, is also rich for any pair of h_1 and h_2. We set $m_k = \|h_k^{(-1)}\|$ and $\tau = \langle h_1^{(-1)}, h_2^{(-1)}\rangle$.

Lemma 2. *Assume that h_1, h_2 are linearly independent functions of zero mean. Then set $\mathcal{R}(h_1, h_2)$ of double zero-range resonance for operator B is the circle*

$$\mathcal{R}(h_1, h_2) = \{\beta \in \mathbb{C}\colon |\beta - \beta_0| = \rho\}$$

in the complex plane, where

$$\beta_0 = \frac{\bar\tau}{m_1^2 m_2^2 - |\tau|^2}, \qquad \rho = \frac{m_1 m_2}{m_1^2 m_2^2 - |\tau|^2}.$$

In addition, if $\beta \in \mathcal{R}(h_1, h_2)$, then the constant function and function

$$\omega_\beta = e^{i\arg(\beta^{-1}+\tau)} m_2 h_1^{(-2)} - m_1 h_2^{(-2)}$$

are two linearly independent half-bound states of B.

Note that circle $\mathcal{R}(h_1, h_2)$ is well defined for linearly independent h_1 and h_2, because then the first antiderivatives $h_1^{(-1)}$ and $h_2^{(-1)}$ are also linearly independent, and $|\tau| < m_1 m_2$ in view of the Cauchy-Schwartz inequality. For instance, if functions $h_1^{(-1)}$ and $h_2^{(-1)}$ are orthonormal, then $\mathcal{R}(h_1, h_2)$ is a unit circle centered at the origin, since $m_1 = m_2 = 1$ and $\tau = 0$. If $h_1^{(-1)}$ and $h_2^{(-1)}$ are simply orthogonal, then $\mathcal{R}(h_1, h_2) = \{\beta \in \mathbb{C}\colon |\beta| = m_1^{-1} m_2^{-1}\}$. In the case when $h_2 = h_1 + \varepsilon g$ and ε is small, that is to say, the angle between h_1 and h_2 is small, the center β_0 is far from the origin and the radius ρ is large, because then the difference $m_1 m_2 - |\tau|$ is of order ε.

Proof: We start with the observation that $\nu = 1$ is obviously a solution of equation

$$-\nu'' + \bar\beta \langle h_2, \nu\rangle h_1 + \beta \langle h_1, \nu\rangle h_2 = 0,$$

since h_k are functions with zero-mean values. For the same reason, the second anti-derivatives $h_k^{(-2)}$ are bounded on the whole line. Then regarding this equation as the "non-homogeneous" one

$$\nu'' = \bar\beta \langle h_2, \nu\rangle h_1 + \beta \langle h_1, \nu\rangle h_2, \tag{3.3}$$

we can look for another half-bound state in the form $\omega = c_1 h_1^{(-2)} + c_2 h_2^{(-2)}$. We do not take into account solution x of the homogeneous equation, because it is unbounded as $|x| \to \infty$.

Since h_1 and h_2 are linearly independent, substituting ω into (3.3) yields

$$\begin{cases} \beta \langle h_1, h_1^{(-2)}\rangle c_1 + (\beta \langle h_1, h_2^{(-2)}\rangle - 1) c_2 = 0, \\ (\bar\beta \langle h_2, h_1^{(-2)}\rangle - 1) c_1 + \bar\beta \langle h_2, h_2^{(-2)}\rangle c_2 = 0. \end{cases} \tag{3.4}$$

Because h_j has compact support, the scalar product $\langle h_j, h_k^{(-2)}\rangle$ is finite, even though antiderivative $h_k^{(-2)}$ does not belong to $L_2(\mathbb{R})$. In addition, the integrating by parts shows $\langle h_j, h_k^{(-2)}\rangle = -\langle h_j^{(-1)}, h_k^{(-1)}\rangle$. Then (3.4) becomes

$$\begin{cases} \beta m_1^2 c_1 + (\beta\tau + 1) c_2 = 0, \\ (\overline{\beta\tau} + 1) c_1 + \bar\beta m_2^2 c_2 = 0. \end{cases} \tag{3.5}$$

This system has a non-trivial solution (c_1, c_2) if and only if $|\beta| m_1 m_2 = |\beta\tau + 1|$. The condition can be written as $|\beta^{-1} + \tau| = m_1 m_2$.

Given $a \in \mathbb{C}$ and $r \in \mathbb{R}$, we consider the circle $\{z \in \mathbb{C}\colon |z - a| = r\}$. Suppose that $|a| < r$. The mapping $z \mapsto z^{-1}$ is a bijection from this circle onto another one

$$\left\{ z \in \mathbb{C}\colon \left| z + \frac{\bar a}{r^2 - |a|^2} \right| = \frac{r}{r^2 - |a|^2} \right\},$$

as is easy to check. Therefore, the resonance region $\mathcal{R}(h_1, h_2)$ arises as the image of the circle $\{z \in \mathbb{C}\colon |z + \tau| = m_1 m_2\}$ under the transformation $z \mapsto z^{-1}$. Note that $|\tau| < m_1 m_2$ by the Cauchy-Schwartz inequality.

If $\beta \in \mathcal{R}(h_1, h_2)$, then (3.5) admits a nontrivial solution having the form

$$c_1 = e^{i\arg(\beta^{-1}+\tau)} m_2, \qquad c_2 = -m_1.$$

In fact, substituting this solution into the first equation yields

$$\begin{aligned} \beta m_1^2 c_1 + (\beta\tau + 1) c_2 &= \beta m_1^2 m_2 e^{i\arg(\beta^{-1}+\tau)} - m_1(\beta\tau + 1) \\ &= \beta m_1 |\beta^{-1} + \tau| e^{i\arg(\beta^{-1}+\tau)} - m_1(\beta\tau + 1) \\ &= \beta m_1(\beta^{-1} + \tau) - m_1(\beta\tau + 1) = 0, \end{aligned}$$

since $m_1 m_2 = |\beta^{-1} + \tau|$. Hence, $\omega_\beta = e^{i\arg(\beta^{-1}+\tau)} m_2 h_1^{(-2)} - m_1 h_2^{(-2)}$ is a half-bound state of B, which is different from the constant one. □

4. PROOF OF MAIN RESULTS

We start with some assertions, which will be used below.

Lemma 3. *Let $\{S_\varepsilon\}_{\varepsilon>0}$ be a family of self-adjoint operators in a Hilbert space $\mathcal{L}$ and $\{W_\varepsilon\}_{\varepsilon>0}$ be a family of unitary operators in $\mathcal{L}$. Assume that $S_\varepsilon \to S$ as $\varepsilon \to 0$ in the norm resolvent sense, $W_\varepsilon \to W$ in the strong operator topology as $\varepsilon \to 0$ and W is a unitary operator in $\mathcal{L}$. Then the family of operators $Q_\varepsilon = W_\varepsilon S_\varepsilon W_\varepsilon^{-1}$ converges in the strong resolvent sense to the operator $Q = WSW^{-1}$ with the domain $\{\phi \in \mathcal{L}\colon W^{-1}\phi \in \operatorname{dom} S\}$.*

Proof: We first note that

$$(Q_\varepsilon-\zeta)^{-1}-(Q-\zeta)^{-1} = W_\varepsilon\big((S_\varepsilon-\zeta)^{-1}-(S-\zeta)^{-1}\big)W_\varepsilon^{-1} + W_\varepsilon(S-\zeta)^{-1}(W_\varepsilon^{-1}-W^{-1}) + (W_\varepsilon - W)(S-\zeta)^{-1}W^{-1},$$

provided $\zeta \in \mathbb{C}\setminus\mathbb{R}$. The operator S is self-adjoint as a limit of self-adjoint operators S_ε in the norm resolvent topology. From the last relation and the self-adjointness of S we have

$$\|(Q_\varepsilon-\zeta)^{-1}f-(Q-\zeta)^{-1}f\| \le \|(S_\varepsilon-\zeta)^{-1}-(S-\zeta)^{-1}\|\,\|f\| + |\operatorname{Im}\zeta|^{-1}\|(W_\varepsilon^{-1}-W^{-1})f\| + \|(W_\varepsilon-W)(S-\zeta)^{-1}W^{-1}f\| \tag{4.1}$$

for all $f \in \mathcal{L}$. The first term in the right-hand side tends to zero as $\varepsilon \to 0$, since operators S_ε converge to S in the norm resolvent sense. The last two terms are infinitely small as $\varepsilon \to 0$, in view of the strong convergence of W_ε. □

We introduce two unitary operators

$$(W_\varepsilon f)(x) = e^{ia\left(\frac{x}{\varepsilon}\right)}f(x), \qquad (Wf)(x) = e^{i\mu H(x)}f(x), \tag{4.2}$$

in $L_2(\mathbb{R})$, where a and μ given by (2.11) and (2.2), respectively, and H is the Heaviside step function

$$H(x) = \begin{cases} 0, & \text{for } x<0,\\ 1, & \text{for } x>0.\end{cases}$$

Lemma 4. *Let W_ε and W be the unitary operators given by (4.2). Then W_ε converge to W as $\varepsilon \to 0$ in the strong operator topology.*

Proof: Without loss of generality we can assume that the support of the magnetic potential A lies in $(-1,1)$. Therefore, $a(\varepsilon^{-1}x)=0$ for $x<-\varepsilon$ and $a(\varepsilon^{-1}x)=\mu$ for $x>\varepsilon$. For each $f \in L_2(\mathbb{R})$ we have

$$\|W_\varepsilon f - Wf\|^2 \le \int_{\mathbb{R}} \left|e^{ia\left(\frac{x}{\varepsilon}\right)} - e^{i\mu H(x)}\right|^2 |f(x)|^2\,dx = \int_{-\varepsilon}^{\varepsilon} \left|e^{ia\left(\frac{x}{\varepsilon}\right)} - e^{i\mu H(x)}\right|^2 |f(x)|^2\,dx \le 4\int_{-\varepsilon}^{\varepsilon}|f(x)|^2\,dx, \tag{4.3}$$

since $a(\varepsilon^{-1}x) = \mu H(x)$ for $|x|>\varepsilon$. The right-hand side of (4.3) tends to zero as $\varepsilon \to 0$, by absolute continuity of the Lebesgue integral. □

4.1. Proof of Theorem 1

Let us consider the Schrödinger operators

$$S_\varepsilon = -\frac{d^2}{dx^2} + V_0(x) + \frac{\alpha}{\varepsilon^2}V\left(\frac{x}{\varepsilon}\right) + \frac{1}{\nu_\varepsilon}U\left(\frac{x}{\nu_\varepsilon}\right), \qquad \operatorname{dom} S_\varepsilon = W_2^2(\mathbb{R}). \tag{4.4}$$

It is of course that S_ε is a version of operator $\mathcal{H}_{\varepsilon\nu}$ given by (2.1) when the magnetic potential is disabled. We also denote by $S = S(\theta,\gamma)$ the Schrödinger operator acting via $S\psi = -\psi'' + V_0\psi$ on functions ψ in $\mathcal{V}$ obeying the interface conditions

$$\begin{pmatrix}\psi(+0)\\ \psi'(+0)\end{pmatrix} = \begin{pmatrix}\theta & 0\\ \gamma & \theta^{-1}\end{pmatrix}\begin{pmatrix}\psi(-0)\\ \psi'(-0)\end{pmatrix} \tag{4.5}$$

at the origin. For all real θ and γ, this operator is self-adjoint.

The proof of Theorem 1 is based on the results obtained in Golovaty [32, 33]. Let $\{\nu_\varepsilon\}_{\varepsilon>0}$ be a sequence such that $\nu_\varepsilon \to 0$ as $\varepsilon \to 0$ and the ratio $\nu_\varepsilon/\varepsilon$ tends to $\lambda \in \Lambda$. If the potential αV is resonant, then the operator family S_ε converges in the norm resolvent sense as $\varepsilon \to 0$ to operator $S = S(\theta(\alpha), \gamma(\alpha,\lambda))$, where θ, γ are given by (2.3)–(2.6). We see at once that operator $\mathcal{H}_{\varepsilon\nu_\varepsilon}$ is unitarily equivalent to operator S_ε, i.e., $\mathcal{H}_{\varepsilon\nu_\varepsilon} = W_\varepsilon S_\varepsilon W_\varepsilon^{-1}$ with the unitary operator (the gauge transformation) W_ε given by (4.2) [28]. For instance, it is easy to check that

$$-e^{ia\left(\frac{x}{\varepsilon}\right)}\frac{d^2}{dx^2}\left(e^{-ia\left(\frac{x}{\varepsilon}\right)}\phi(x)\right) = \left(i\frac{d}{dx} + \frac{1}{\varepsilon}A\left(\frac{x}{\varepsilon}\right)\right)^2\phi(x),$$

since $a' = A$. Next, $W^{-1}(\operatorname{dom}\mathcal{H}) \subset \operatorname{dom} S$, where $W^{-1}f = e^{-i\mu H}f$. In fact, given $\phi \in \operatorname{dom}\mathcal{H}$, we set $\psi = W^{-1}\phi = e^{-i\mu H}\phi$. Then we have $\psi(+0) = e^{-i\mu}\phi(+0)$, $\psi'(+0) = e^{-i\mu}\phi'(+0)$, $\psi(-0) = \phi(-0)$ and $\psi'(-0) = \phi'(-0)$. Rewriting conditions (2.7) for ϕ in the form

$$\begin{pmatrix}e^{-i\mu}\phi(+0)\\ e^{-i\mu}\phi'(+0)\end{pmatrix} = \begin{pmatrix}\theta(\alpha) & 0\\ \gamma(\alpha,\lambda) & \theta(\alpha)^{-1}\end{pmatrix}\begin{pmatrix}\phi(-0)\\ \phi'(-0)\end{pmatrix},$$

we ascertain that ψ satisfies (4.5) and therefore $\psi \in \operatorname{dom} S$. Obviously,

$$W^{-1}\colon \operatorname{dom}\mathcal{H} \to \operatorname{dom} S$$

is a linear isomorphism. Therefore, the limit operator $\mathcal{H}$ in Theorem 1 can be written as $\mathcal{H} = WSW^{-1}$.

In view of Lemma 4, the gauge transformations W_ε converge to W in the strong operator topology. Since the resolvents of S_ε converge to the resolvent of S uniformly, we deduce from Lemma 3 that

$$\mathcal{H}_{\varepsilon\nu_\varepsilon} = W_\varepsilon S_\varepsilon W_\varepsilon^{-1} \to WSW^{-1} = \mathcal{H} \qquad \text{as } \varepsilon \to 0$$

in the strong resolvent sense.

4.2. Proof of Theorem 2

We can now argue almost exactly as in the proof of Theorem 1. First of all note that operators $\mathcal{T}_\varepsilon$ given by (4.6) are unitarily equivalent to operators

$$T_\varepsilon = -\frac{d^2}{dx^2} + V_0(x) + \frac{1}{\varepsilon^3}\, G_\varepsilon + \frac{1}{\varepsilon}\, U\Big(\frac{x}{\varepsilon}\Big), \qquad (4.6)$$

namely $\mathcal{T}_\varepsilon = W_\varepsilon T_\varepsilon W_\varepsilon^{-1}$ with the gauge transformation W_ε given by (4.2). Operator $G_\varepsilon = G_\varepsilon(g_1, g_2)$ is a rank-two operator of the form

$$(G_\varepsilon\psi)(x) = \bar\beta\, \langle g_2(\varepsilon^{-1}\cdot), \psi\rangle\, g_1(\varepsilon^{-1}x) + \beta\, \langle g_1(\varepsilon^{-1}\cdot), \psi\rangle\, g_2(\varepsilon^{-1}x),$$

where $g_1 = e^{-ia} f_1$ and $g_2 = e^{-ia} f_2$ are the same functions as in (2.12). In fact, a trivial verification shows that $F_\varepsilon = W_\varepsilon G_\varepsilon W_\varepsilon^{-1}$.

In Theorem 2 we assumed g_1, g_2 were linearly independent functions of zero mean. Moreover, $a_2 \neq \bar\varkappa a_1$. It has recently been proved in Golovaty [26] that if additionally coupling constant β belongs to the set $\mathcal{R}(g_1, g_2)$ of double zero-energy resonance for $B = -\frac{d^2}{dx^2} + \bar\beta\, \langle g_2, \cdot\rangle\, g_1 + \beta\, \langle g_1, \cdot\rangle\, g_2$, then operators T_ε converge as $\varepsilon \to 0$ in the norm resolvent sense to operator $T\psi = -\psi'' + V_0\psi$ acting on functions $\psi \in \mathcal{V}$ obeying the interface conditions

$$\begin{pmatrix}\psi(+0)\\ \psi'(+0)\end{pmatrix} = e^{i\arg(a_2 - \varkappa\bar a_1)} \begin{pmatrix} \dfrac{|\varkappa|^2 a_0 - 2\mathrm{Re}(\overline{\varkappa} a_1) + a_2}{|a_2 - \overline{\varkappa} a_1|} & \dfrac{|\varkappa|^2}{|a_2 - \overline{\varkappa} a_1|} \\ \dfrac{a_0 a_2 - |a_1|^2}{|a_2 - \overline{\varkappa} a_1|} & \dfrac{a_2}{|a_2 - \overline{\varkappa} a_1|} \end{pmatrix} \begin{pmatrix}\psi(-0)\\ \psi'(-0)\end{pmatrix}$$

at the origin. Therefore, $\mathcal{T} = WTW^{-1}$, by reasoning similar to that in the proof of Theorem 1. We can now repeatedly apply Lemma 3 for operator families $\{T_\varepsilon\}_{\varepsilon>0}$ and $\{W_\varepsilon\}_{\varepsilon>0}$ to deduce the strong resolvent convergence

$$\mathcal{T}_\varepsilon = W_\varepsilon T_\varepsilon W_\varepsilon^{-1} \to WTW^{-1} = \mathcal{T}$$

as $\varepsilon \to 0$.

5. FINAL REMARKS

In Theorem 1 we obtained in the limit the coupling conditions

$$\begin{pmatrix}\phi(+0)\\ \phi'(+0)\end{pmatrix} = e^{i\mu(A)} \begin{pmatrix} \theta(V) & 0 \\ \gamma(V,U) & \theta^{-1}(V) \end{pmatrix} \begin{pmatrix}\phi(-0)\\ \phi'(-0)\end{pmatrix},$$

in which the magnetic potential A appeared only in the phase factor $e^{i\mu(A)}$. This situation is typical for potential perturbations of Schrödinger operators.

Unlike the previous case, in which the potential perturbation was invariant with respect to the gauge transformation W_ε, the finite-rank perturbation F_ε is not invariant. In fact, $F_\varepsilon = W_\varepsilon G_\varepsilon W_\varepsilon^{-1}$; transformation W_ε rotates the plane $\mathrm{span}\{f_1, f_2\}$ when we change parameter ε. This is certainly the main reason why the magnetic field A has an effect on all coefficients in the coupling conditions

$$\begin{pmatrix}\phi(+0)\\ \phi'(+0)\end{pmatrix} = e^{i\mu(A)} \begin{pmatrix} c_{11}(A) & c_{12}(A) \\ c_{21}(A) & c_{22}(A) \end{pmatrix} \begin{pmatrix}\phi(-0)\\ \phi'(-0)\end{pmatrix}$$

appearing as the solvable model in Theorem 2. Of course, the coefficients c_{kj} depend on potentials V, U and functions f_1, f_2 too.

AUTHOR CONTRIBUTIONS

The author confirms being the sole contributor of this work and has approved it for publication.

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A Perturbative Approach to the Tunneling Phenomena

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The double-well potential is a good example, where we can compute the splitting in the bound state energy of the system due to the tunneling effect with various methods, namely path-integral, WKB, and instanton calculations. All these methods are non-perturbative and there is a common belief that it is difficult to find the splitting in the energy due to the barrier penetration from a perturbative analysis. However, we will illustrate by explicit examples including singular potentials (e.g., Dirac delta potentials supported by points and curves and their relativistic extensions) it is possible to find the splitting in the bound state energies by developing some kind of perturbation method.

Keywords: Dirac delta potentials, Krein's formulae, resolvent, perturbation theory, tunneling, Dirac delta potentials supported by curves, heat kernel, bound state energy

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1. INTRODUCTION

Most real quantum mechanical systems can not be solved exactly and we usually apply some approximation methods, the most common one being perturbation theory, to get information about the energy levels and scattering amplitudes. However, not all quantum systems can be analyzed by perturbative methods. There are various class of problems where we can not deduce any information by simply using perturbation theory since these problems are inherently non-perturbative phenomena like the formation of bound states and penetration through a potential barrier. For such non-perturbative phenomenon, other tools, such as WKB [1, 2] and instanton calculations [3], are particularly useful. The particle moving in a one-dimensional anharmonic potential $V(x) = \frac{\lambda^2}{8}(x^2 - a^2)^2$ is a classic example, where we can show the barrier penetration through the WKB analysis.

When the energy scale determined by the length scale a is extremely small compared with the binding energy of the system, i.e., $\hbar^2/2ma^2 << E_B$, or $\lambda a^2 >> 1$, the potential separates into two symmetrical wells with a very high barrier (see **Figure 1**). In this extreme regime, as a first approximation, each well has separately quantized energy levels and these energy levels are degenerate due to the symmetry. However, once the large but finite value of the coupling constant λ is taken into account, the particle initially confined to one well can tunnel to the other well so the degeneracy in the energy levels disappear. The splitting in the resulting energy levels (between the true ground state and the first excited level due to the tunneling) is given by Landau [1] and Das [2]

$$\delta E = E_2 - E_1 \approx \frac{4e}{\pi}\sqrt{m\hbar}\omega^{3/2} a \exp\left(-\frac{1}{\hbar}S_0\right) \tag{1}$$

where $S_0 = \frac{2m\omega a^2}{3}$ and $\omega^2 = \frac{\lambda^2 a^2}{m}$. The above exponentially decaying factor with respect to the separation between the wells illustrates the tunneling effect. The true ground state corresponds to

a symmetric combination and the excited level corresponds to the anti-symmetric combination of the WKB corrected wave functions.

Among the exactly solvable potentials in quantum mechanics, Dirac delta well potentials are the most well-known text book example [4]. Moreover, it has been studied extensively in mathematical physics literature from the different point of views, in particular in the context of self-adjoint extension of symmetric operators [5]. Although it is easier to define it rigorously in one dimension through the quadratic forms, one possible way to define it in higher dimensions is to consider the free symmetric Hamiltonian defined on a dense domain excluding the point, where the support of the Dirac delta function is located, and then apply the self-adjoint extension techniques developed by J. Von Neumann [see the monograph [6] for the details and also for the historical development with extensive literature in the subject]. Then, the formal (or heuristic) definition of one-dimensional Dirac delta potentials in the physics literature is understood as the one particular choice among the four parameter family of the self-adjoint operators, where the matching conditions of the wave function are just obtained from the boundary conditions (which define the domain of our self-adjoint operator) constructed through the extension theory. Another way to introduce these point interactions uses the resolvent method, developed by M. Krein, and it is based on the observation that for such type of potentials the resolvent can be found explicitly and expressed via the so-called Krein's formula [7]. Within this approach, the Hamiltonian for point interaction (in two and three dimensions) is first approximated (regularized) by a properly chosen sequence of self-adjoint operators H_ϵ and then the coupling constant (or strength) of the potential is assumed to be a function of the parameter ϵ in such a way that one obtains a non-trivial limit. This convergence is actually in the strong resolvent sense, so the limit operator is self-adjoint [8]. Since the Dirac delta potentials in two and three dimensions require renormalization, it is usually considered as a toy model for the renormalization originally developed in quantum field theories and it helps us to better understand the various ideas in field theory such as renormalization group and asymptotic freedom [9–12]. Furthermore, point like Dirac delta interactions have been also extended to various generalizations. For our approach, to illustrate the main ideas, we are mainly concerned with the delta potentials supported by points on flat and hyperbolic manifolds [13–15], and delta potentials supported by curves in flat spaces, and its various relativistic extensions in flat spaces [16–19].

In this paper, we explicitly demonstrate for a class of singular potential problems that the splitting in the energy levels due to the tunneling can be realized by simply developing some kind of perturbation theory. We have two basic assumptions here: (1) Binding energies of individual Dirac delta potentials are all different. Otherwise we need to employ degenerate perturbation theory. Actually, we briefly discus a particular degenerate case, namely the two center case in two dimensions to compare with the double well potential. (2) The support of singular interactions are sufficiently separated from one another, as a result the bound state wave functions decay rapidly over the distances between them.

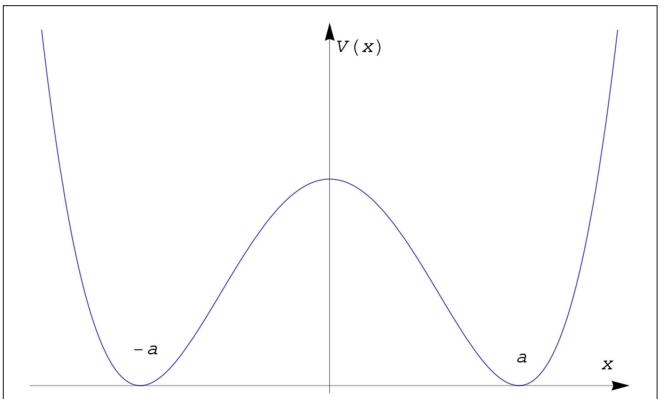

FIGURE 1 | Anharmonic potential.

All the findings about the splitting in the bound state energies for singular potentials on hyperbolic manifolds treated here could be applied to the two dimensional systems such as graphite sheets. We can model impurities in these systems as attractive centers in some approximation and these sheets can be put in various shapes. This is especially true for surfaces with variable sectional curvature which is not completely negative. The negatively curved surfaces, of course, cannot be realized as embedded surfaces in three dimensions due to Hilbert's well-known theorem. Nevertheless, we may envisage these models as an effective description of unusual quasi-particle states of some two dimensional systems. Due to the interactions, the system may develop a gap in the spectrum and the effective description may well be best understood through a negative sectional curvature space. Moreover, the problems related with point interactions on Lobachevsky plane have been studied from different points of view [20, 21]. The point interactions can be extended on more general class of manifolds as well [22]. In particular, they have been studied on some particular surfaces in $\mathbb{R}^3$, namely on the infinite planar strip as a natural model for quantum wires containing impurities [23] and on the torus [24]. A more heuristic approach for point interactions on Riemannian manifolds has been constructed through the heat kernel in Altunkaynak et al. [13] and Erman and Turgut [14]. The physical motivation behind studying the Dirac delta potentials supported by curves is based on the need for modeling semiconductor wires [25]. They could be considered as a toy model for electrons confined to narrow tube-like regions.

The paper is organized as follows: In section 2, we formally summarize the resolvent formulae, called Krein's formulae, for Hamiltonians perturbed by singular potentials including Dirac delta potentials supported by points and curves. The principal matrices for each case are given explicitly. The relativistic and the field theoretical extension of it has been also reviewed in the subsections of this section. In section 3, we briefly discuss the analytic structure of the principal matrix and the bound state spectrum for such type of singular interactions.

In Section 4, we discuss how the off-diagonal terms of the principal matrix change in the tunneling regime. section 5 and section 6 contain the formulation of the perturbative analysis and explicit calculations of the splitting in the bound state energy when these singular interactions are far away from each other, which is the main result of the paper. We finally discuss the degenerate case and wave functions, and compare the one dimensional results with the exact result in section 7.

2. KREIN'S FORMULAE FOR FREE HAMILTONIANS PERTURBED BY SINGULAR INTERACTIONS

Before we are going to discuss the perturbative analysis of singular interactions *for large separations of the support of the potentials*, we first present the basic results about our formulation of the singular Hamiltonians. In this paper, we are mainly concerned with the Dirac delta potentials supported by finitely many points and finitely many curves in flat spaces, and their extension to the hyperbolic manifolds. Moreover, we also consider some relativistic extensions of these singular interactions.

Since we study the spectral properties of different kinds of Dirac delta potentials, we first introduce the notation for Dirac delta functions of interest. The Dirac delta distribution δ_a supported by a point $\mathbf{a}$ in $\mathbb{R}^n$ is defined as a continuous linear functional whose action on the test functions ψ is given by

$$\langle \delta_a, \psi \rangle = \psi(\mathbf{a}) \, . \tag{2}$$

Similarly, Dirac delta distribution δ_γ supported by a curve Γ in $\mathbb{R}^n$ is defined as a continuous linear functional whose action on the test functions ψ is given by Appel [26]

$$\langle \delta_\gamma, \psi \rangle = \int_\Gamma ds \; \psi(\gamma(s)) \, . \tag{3}$$

The left hand sides in the definitions (2) and (3) can be expressed in the Dirac's bra-ket notation, most common in physics literature, as $\langle \mathbf{a}|\psi\rangle$ and $\langle \gamma|\psi\rangle$, respectively.

As we have already emphasized in the introduction, there are several ways to define rigorously the Hamiltonian for Dirac delta potentials. Here, we start with a finite rank perturbations of self-adjoint free Hamiltonian H_0 (e.g., $H_0 = P^2/2m$ in the non-relativistic case and $H_0 = \sqrt{P^2 + m^2}$ in the semi-relativistic case):

$$H = H_0 - \sum_{i=1}^{N} \lambda_i \langle \varphi_i, . \rangle \; \varphi_i \, , \tag{4}$$

where $\varphi_i \in \mathcal{H}$ and $\langle ., . \rangle$ denotes the sesqui-linear inner product in the Hilbert space $\mathcal{H}$. Then, it is well-known that the resolvent of H can be explicitly found in terms of the resolvent of the free part by simply solving the inhomogenous equation [7]

$$(H - z)\psi = \rho \, , \tag{5}$$

for a given $\rho \in \mathcal{H}$ and $\psi \in D(H_0) = D(H)$. Here D stands for the domain of the operator and we assume that $\Im(z) > 0$. It is well-known that H is self-adjoint on $D(H_0)$ due to the Kato-Rellich theorem [5]. The resolvent of H could be found in two steps: First, we apply the resolvent of the free part to the Equation (5)

$$(H_0 - z)^{-1}\rho = \psi - \sum_{i=1}^{N} \lambda_i \langle \varphi_i, \psi \rangle \; (H_0 - z)^{-1}\varphi_i \, , \tag{6}$$

and project this on the vector φ_j, we can then find the solution $\langle \varphi_i, \psi \rangle$ so that the resolvent $R_z(H) = (H - z)^{-1}$ of the Hamiltonian H at z is:

$$R_z(H) = R_z(H_0) + \sum_{i,j=1}^{N} R_z(H_0)\varphi_i \; [\Phi^{-1}(z)]_{ij} \; \langle R_{\bar{z}}(H_0)\varphi_j, . \rangle \, , \tag{7}$$

where

$$\Phi_{ij}(z) = \begin{cases} \frac{1}{\lambda_i} - \langle \varphi_i, R_z(H_0)\varphi_i \rangle & \text{if } i = j \\ -\langle \varphi_i, R_z(H_0)\varphi_j \rangle & \text{if } j \neq j' \end{cases} \, . \tag{8}$$

Actually, the resolvent formula (7) is valid even in the case where the vectors φ_i's do not belong to the Hilbert space. Such perturbations represent the singular type of interactions, e.g., Dirac delta potentials supported by points or curves [6, 16]. In Dirac's bra-ket notation, one can also express the above resolvent formula as:

$$R_z(H) = R_z(H_0) + \sum_{i,j=1}^{N} R_z(H_0)|\varphi_i\rangle \; [\Phi^{-1}(z)]_{ij} \; \langle \varphi_j|R_z(H_0) \, . \tag{9}$$

The explicit expression of the resolvent (7) or (9) is known as Krein's resolvent formula. Alternatively, these singular interactions can be defined directly through von Neumann's self-adjoint extension theory (or quadratic forms in some cases). Since our aim is the spectral behavior and especially the bound state problem of such singular interactions, Krein's explicit formula is much more useful. Throughout the paper, following the terminology introduced by Rajeev [27] we call the matrix Φ as the principal matrix (this is equivalent to the matrix Γ used in Albeverio et al. [6]).

Actually, one can also develop the above resolvent formula (9) to relativistic and field theoretical extensions of the singular models, as we will discuss in the next subsections. Let us now summarize explicitly the resolvent formulae and principal matrices in all classes of singular interactions that we are going to discuss in this paper:

2.1. Point-Like Dirac Delta Interactions in $\mathbb{R}$

The Hamiltonian for the non-relativistic particle moving in fixed N point like Dirac delta potentials in one dimension can be expressed in terms of the formal projection operators given by the Dirac kets $|a_i\rangle$

$$H = H_0 - \sum_{i=1}^{N} \lambda_i |a_i\rangle\langle a_i| \,, \tag{10}$$

where H_0 is the non-relativistic free Hamiltonian, and λ_j's are positive constants, called coupling constants or strengths of the potential. Throughout this paper, *we will use the units such that* $\hbar = 2m = 1$ *for non-relativistic cases and* $\hbar = c = 1$ *only for the relativistic case*. Since we have fairly complicated expressions, this simplifies our writing, hoping that this does not lead to any further complications. It is well-known in the literature that there are different ways to make sense of this formal Hamiltonian in a mathematically rigorous way [strictly speaking, the above expression (10) has no meaning as an operator in $L^2(\mathbb{R})$]. Let us define $R_z(H) := R(z)$ and $R_z(H_0) := R_0(z)$ for simplicity. Even though it is hard to make sense of the Hamiltonian, one can find the resolvent of this formal operator algebraically and the result is consistent with the one given by a more rigorous formulation. Choosing φ_i as the Dirac kets $|a_i\rangle$ formally in the previous section, the resolvent is explicitly given by

$$R(z) = R_0(z) + \sum_{i,j=1}^{N} R_0(z)|a_i\rangle [\Phi^{-1}(E)]_{ij} \langle a_j| R_0(z) \,, \tag{11}$$

where Φ is an $N \times N$ matrix

$$\Phi_{ij}(z) = \begin{cases} \frac{1}{\lambda_i} - R_0(a_i, a_i; z) & \text{if } i = j \\ -R_0(a_i, a_j; z) & \text{if } i \neq j \end{cases} . \tag{12}$$

Here $R_0(a_i, a_j; z) = \langle a_i|(H_0 - z)^{-1}|a_j\rangle$ is the free resolvent kernel. It is useful to express the principal matrix in terms of the heat kernel $K_t(a_i, a_j)$ - the fundamental solution to the Cauchy problem associated with the heat equation—using

$$\begin{aligned} R_0(a_i, a_j; z) &= \langle a_i|(H_0 - z)^{-1}|a_j\rangle = \langle a_i| \int_0^\infty dt\, e^{t(H_0 - z)}|a_j\rangle \\ &= \int_0^\infty dt\; K_t(a_i, a_j)\, e^{tz} \,. \end{aligned} \tag{13}$$

Then, we obtain

$$\Phi_{ij}(z) = \begin{cases} \frac{1}{\lambda_i} - \int_0^\infty dt\, K_t(a_i, a_i) e^{tz} & \text{if } i = j \\ -\int_0^\infty dt\, K_t(a_i, a_j) e^{tz} & \text{if } i \neq j \end{cases} . \tag{14}$$

These expressions should be considered as analytical continuations of the formulae beyond their regions of convergence in the variable z. From the resolvent (11), one can also write down the resolvent kernel

$$R(x_1, x_2; z) = R_0(x_1, x_2; z) + \sum_{i,j=1}^{N} R_0(x_1, a_i; z)[\Phi^{-1}]_{ij} R_0(a_j, x_2; z) \,. \tag{15}$$

Using the explicit expression of the integral kernel of the free resolvent

$$R_0(x, y; z) = \frac{i}{2\sqrt{z}}\, e^{i\sqrt{z}|x-y|} \,, \tag{16}$$

we have

$$\Phi_{ij}(z) = \begin{cases} \frac{1}{\lambda_i} - \frac{i}{2\sqrt{z}} & \text{if } i = j \\ -\frac{i}{2\sqrt{z}}\, e^{i\sqrt{z}|a_i - a_j|} & \text{if } i \neq j \end{cases} . \tag{17}$$

Here $\sqrt{z}$ is defined as the unambiguous square root of z with $\Im\sqrt{z}$ is positive. Since we study the bound state spectrum, it is sometimes convenient to express the above matrix $\Phi(z)$ in terms of a real positive variable $\nu = -i\sqrt{z}$, i.e.,

$$\Phi_{ij}(z)\Big|_{z=-\nu^2} := \Phi_{ij}(\nu) = \begin{cases} \frac{1}{\lambda_i} - \frac{1}{2\nu} & \text{if } i = j \\ -\frac{1}{2\nu}\, e^{-\nu|a_i - a_j|} & \text{if } i \neq j \end{cases} . \tag{18}$$

2.2. Point-Like Dirac Delta Interactions in $\mathbb{R}^2$ and $\mathbb{R}^3$

We assume that the centers of the Dirac delta potentials do not coincide, that is, $\mathbf{a}_i \neq \mathbf{a}_j$ whenever $i \neq j$. If we follow the same steps outlined above, we find exactly the same formal expression for the resolvent for point interactions in two and three dimensions except for the fact that the explicit expression of the integral kernel of the free resolvent in $\mathbb{R}^2$ and $\mathbb{R}^3$ [6] are given by

$$R_0(\mathbf{r_1}, \mathbf{r_2}; z) = \frac{i}{4}\, H_0^{(1)}(\sqrt{z}|\mathbf{r_1} - \mathbf{r_2}|) \,, \tag{19}$$

$$R_0(\mathbf{r_1}, \mathbf{r_2}; z) = \frac{e^{i\sqrt{z}|\mathbf{r_1} - \mathbf{r_2}|}}{4\pi\,|\mathbf{r_1} - \mathbf{r_2}|} \,, \tag{20}$$

respectively. Here $H_0^{(1)}$ is the Hankel function of the first kind of order zero and $\Im\sqrt{z} > 0$. Unfortunately, the diagonal part of the free resolvent kernels are divergent so the diagonal part of the principal matrices are infinite. This is clear for the three dimensional case from the asymptotic behavior of the Hankel function [28]

$$H_0^{(1)}(x) \approx -\frac{2i}{\pi} \log(2/x) \,, \tag{21}$$

as $x \to 0$.

This difficulty can be resolved by the so-called regularization and renormalization method. Instead of starting with the higher dimensional version of the formal Hamiltonian (10), we first consider the regularized Hamiltonian through the heat kernel

$$H_\epsilon = H_0 - \sum_{i=1}^{N} \lambda_i(\epsilon)\; |\mathbf{a}_i^\epsilon\rangle\langle \mathbf{a}_i^\epsilon| \,, \tag{22}$$

where $\langle \mathbf{r}|\mathbf{a_i}^\epsilon\rangle = K_{\epsilon/2}(\mathbf{r}, \mathbf{a_i})$. The heat kernel associated with the heat equation $\nabla^2\psi - \frac{\partial\psi}{\partial t} = 0$ in $\mathbb{R}^n$ is given by

$$K_t(\mathbf{r_1}, \mathbf{r_2}) = \frac{1}{(4\pi t)^{n/2}} e^{-\frac{|\mathbf{r_1} - \mathbf{r_2}|^2}{4t}} \,. \tag{23}$$

It is important to note that

$$K_{\epsilon/2}(\mathbf{r},\mathbf{a_i}) \to \delta(\mathbf{r}-\mathbf{a_i})\,, \tag{24}$$

as $\epsilon \to 0^+$ in the distributional sense. Then, we can easily find the resolvent kernel associated with the regularized Hamiltonian (22)

$$R_\epsilon(\mathbf{r_1},\mathbf{r_2};z) = R_0(\mathbf{r_1},\mathbf{r_2};z) + \sum_{i,j=1}^{N} R_0(\mathbf{r_1},\mathbf{a_i};z)\left[\Phi_\epsilon(z)\right]^{-1}_{ij} R_0\left(\mathbf{a_j},\mathbf{r_2};z\right), \tag{25}$$

where

$$[\Phi_\epsilon(z)]_{ij} = \begin{cases} \frac{1}{\lambda_i(\epsilon)} - \int_0^\infty dt\; K_{t+\epsilon}(\mathbf{a_i},\mathbf{a_i})\; e^{tz} & \text{if } i=j \\ -\int_0^\infty dt\; K_{t+\epsilon}(\mathbf{a_i},\mathbf{a_j})\; e^{tz} & \text{if } i\neq j \end{cases}. \tag{26}$$

If we choose

$$\frac{1}{\lambda_i(\epsilon)} = \int_0^\infty dt\; K_{t+\epsilon}(\mathbf{a_i},\mathbf{a_i})\; e^{tE_B^i} \tag{27}$$

where $E_B^i < 0$ (the spectrum of the free Hamiltonian only includes the continuous spectrum: $[0,\infty]$) is the bound state energy of the particle to the i th center *in the absence of all the other centers* and take the formal limit $\epsilon \to 0^+$ we find

$$R(\mathbf{r_1},\mathbf{r_2};z) = R_0(\mathbf{r_1},\mathbf{r_2};z) + \sum_{i,j=1}^{N} R_0(\mathbf{r_1},\mathbf{a_i};z)\left[\Phi(z)\right]^{-1}_{ij} R_0\left(\mathbf{a_j},\mathbf{r_2};z\right), \tag{28}$$

where

$$\Phi_{ij}(z) = \begin{cases} \int_0^\infty dt\; K_t(\mathbf{a_i},\mathbf{a_i})\; \left(e^{tE_B^i} - e^{tz}\right) & \text{if } i=j \\ -\int_0^\infty dt\; K_t(\mathbf{a_i},\mathbf{a_j})\; e^{tz} & \text{if } i\neq j \end{cases}. \tag{29}$$

From the explicit form of the heat kernel formula (23), we obtain

$$\Phi_{ij}(z) = \begin{cases} \frac{1}{2\pi}\log\left(-i\sqrt{z/|E_B^i|}\right) & \text{if } i=j \\ -\frac{i}{4}H_0^{(1)}(\sqrt{z}|\mathbf{a_i}-\mathbf{a_j}|) & \text{if } i\neq j \end{cases}, \tag{30}$$

in two dimensions and

$$\Phi_{ij}(z) = \begin{cases} \frac{\left(-i\sqrt{z}-\sqrt{|E_B^i|}\right)}{4\pi} & \text{if } i=j \\ -\frac{e^{i\sqrt{z}|\mathbf{a_i}-\mathbf{a_j}|}}{4\pi|\mathbf{a_i}-\mathbf{a_j}|} & \text{if } i\neq j \end{cases}, \tag{31}$$

in three dimensions.

Since we deal with the bound states in this paper, it is convenient to express the principal matrices in terms of the real positive variable $\nu = -i\sqrt{z}$:

$$\Phi_{ij}(z)|_{z=-\nu^2} = \begin{cases} \frac{1}{2\pi}\log\left(\nu/\sqrt{|E_B^i|}\right) & \text{if } i=j \\ -\frac{1}{2\pi}K_0(\nu|\mathbf{a_i}-\mathbf{a_j}|) & \text{if } i\neq j \end{cases}, \tag{32}$$

in two dimensions and

$$\Phi_{ij}(z)|_{z=-\nu^2} = \begin{cases} \frac{\left(\nu-\sqrt{|E_B^i|}\right)}{4\pi} & \text{if } i=j \\ -\frac{e^{-\nu|\mathbf{a_i}-\mathbf{a_j}|}}{4\pi|\mathbf{a_i}-\mathbf{a_j}|} & \text{if } i\neq j \end{cases}, \tag{33}$$

in three dimensions. Here we have used $K_0(z) = \frac{i\pi}{2}H_0^1(iz)$ with $-\pi < arg(z) < \pi/2$ and $K_0(z)$ is the modified Bessel function of the third kind [28].

2.3. Point-Like Dirac Delta Interactions in $\mathbb{H}^2$ and $\mathbb{H}^3$

Here we assume that the particle is intrinsically moving in the manifold. Our heuristic approach to study such type of interactions on Riemannian manifolds is based on the idea of using the heat kernel as a regulator for point interactions on manifolds [13, 14]. Thanks to the fact (24), the regularized interaction is chosen as the heat kernel on Riemannian manifolds. Once we have regularized the Hamiltonian, one can follow essentially the same steps outlined in the previous section, and obtain exactly the same form of the resolvent and principal matrix as in (28) and (29), respectively. In this paper, we only consider the particular class of Riemannian manifolds, namely two and three dimensional hyperbolic manifolds for simplicity. The heat kernel on hyperbolic manifolds of constant sectional curvature $-\kappa^2$ can be analytically calculated and given by Grigoryan [29]

$$K_t(x,y) = \begin{cases} \frac{\sqrt{2}}{\kappa}\frac{1}{(4\pi t)^{3/2}}\; e^{-\kappa^2 t/4}\int_{\kappa d(x,y)}^\infty ds\; \frac{s\; e^{-s^2/4\kappa^2 t}}{\sqrt{\cosh s - \cosh \kappa d(x,y)}} & \text{for } n=2 \\ \frac{\kappa\, d(x,y)}{(4\pi t)^{3/2}\sinh \kappa d(x,y)}\; e^{-\kappa^2 t - \frac{d^2(x,y)}{4t}} & \text{for } n=3\,, \end{cases} \tag{34}$$

where $d(x,y)$ is the geodesic distance between the points x and y on the manifold. The explicit form of the principal matrix in $\mathbb{H}^3$ can then be easily evaluated [15]:

$$\Phi_{ij}(z) = \begin{cases} \frac{1}{4\pi}\left(\sqrt{\kappa^2-z} - \sqrt{\kappa^2 - E_B^i}\right) & \text{if } i=j \\ -\left(\frac{\kappa\exp\left(-d(a_i,a_j)\sqrt{\kappa^2-z}\right)}{4\pi\sinh\left(\kappa\, d(a_i,a_j)\right)}\right) & \text{if } i\neq j\,. \end{cases} \tag{35}$$

Similarly, the principal matrix in $\mathbb{H}^2$ can simply be evaluated by interchanging the order of integration with respect to t and s

$$\Phi_{ij}(z) = \begin{cases} \frac{1}{2\pi}\left[\psi\left(\frac{1}{2}+\sqrt{-\frac{z}{\kappa^2}+\frac{1}{4}}\right)-\psi\left(\frac{1}{2}+\sqrt{-\frac{E_B^i}{\kappa^2}+\frac{1}{4}}\right)\right] & \text{if } i=j \\ -\frac{1}{2\pi}\, Q_{\frac{1}{2}+\sqrt{-\frac{z}{\kappa^2}+\frac{1}{4}}}\left(\cosh(\kappa\, d(a_i,a_j))\right) & \text{if } i\neq j\,, \end{cases} \tag{36}$$

where ψ is the digamma function with its integral representation [28]

$$\psi(w) = \int_0^\infty \left(\frac{e^{-t}}{t} - \frac{e^{-tw}}{1-e^{-t}}\right) dt\,, \tag{37}$$

for $\Re(w) > 0$, and Q is the Legendre function of second type [28] with its integral representation

$$Q_\alpha(\cosh a) = \int_a^\infty \frac{e^{-(\alpha+\frac{1}{2})r}}{\sqrt{2\cosh r - 2\cosh a}}\, dr\,, \tag{38}$$

for real and positive a and $\Re(\alpha) > -1$.

Since the spectrum of the free Hamiltonian in $\mathbb{H}^n$ includes only the continuous part starting from $(n-1)^2\kappa^2/4$, it is natural to assume $E_B^i < (n-1)^2\kappa^2/4$.

2.4. Two Types of Relativistic Extensions of Point-Like Dirac Delta Interactions

We first consider the so-called semi-relativistic Salpeter type free Hamiltonian (also known as relativistic spin zero Hamiltonian) perturbed by point like Dirac delta potentials in one dimension. This problem for the single center case has been first studied in Albeverio and Kurasov [30] from the self-adjoint extension point of view. The formal Hamiltonian is exactly in the same form as in (10), except for the free part

$$H = \sqrt{-\frac{d^2}{dx^2}+m^2} - \sum_{i=1}^N \lambda_i |a_i\rangle\langle a_i|\,, \tag{39}$$

in the units where $\hbar = c = 1$. This non-local operator is a particular case of pseudo-differential operators and defined in momentum space as multiplication by $\sqrt{p^2+m^2}$ [31], which is known as the symbol of the operator. After following the renormalization procedure outlined above for the point interactions in two and three dimensions, the resolvent and the principal matrix is exactly the same form as in (28) and (29), respectively. However, the explicit expression of the heat kernel in this case is given by Lieb and Loss [31]

$$K_t(x,y) = \frac{mt}{\pi\sqrt{(x-y)^2+t^2}} K_1\left(m\sqrt{(x-y)^2+t^2}\right)\,, \tag{40}$$

where K_1 is the modified Bessel function of the first kind. Due to the short-time asymptotic expansion

$$K_1(mt) \sim \frac{1}{mt}\,, \tag{41}$$

the diagonal term in the principal matrix (29) is divergent. In contrast to the one-dimensional case for point Dirac delta potentials, this problem therefore requires renormalization, as noticed by Erman et al. [18] and Al-Hashimi et al. [32]. Choosing the coupling constants as in (27) by substituting the heat kernel (40) and taking the limit $\epsilon \to 0^+$, we obtain the resolvent in the form of the Krein's formula (11). The explicit form of the diagonal principal matrix is given by Erman et al. [18]

$$\Phi_{ii}(z) = \varphi(E_B^i) - \varphi(z)\,, \tag{42}$$

where

$$\varphi(z) = \frac{z}{\pi\sqrt{m^2-z^2}}\left(\frac{\pi}{2} + \arctan\frac{z}{\sqrt{m^2-z^2}}\right)\,. \tag{43}$$

Its off-diagonal part is given by

$$\Phi_{ij}(z) = \begin{cases} -\frac{1}{\pi}\int_m^\infty d\mu\; e^{-\mu|a_i-a_j|}\frac{\sqrt{\mu^2-m^2}}{\mu^2-m^2+z^2} & \text{if } \Re z < 0 \\ -i\frac{e^{i\sqrt{z^2-m^2}|a_i-a_j|}}{\sqrt{1-\frac{m^2}{z^2}}} - \frac{1}{\pi}\int_m^\infty d\mu\; e^{-\mu|a_i-a_j|}\frac{\sqrt{\mu^2-m^2}}{\mu^2-m^2+z^2} & \text{if } \Re z > 0 \end{cases}\,, \tag{44}$$

where E_B^i is the bound state energy to the i th center in the absence of all the other centers. Since the spectrum of the free Hamiltonian includes only the continuous spectrum starting from m, it is natural to expect that $E_B^i < m$.

An alternative relativistic model can be introduced from a field theory perspective in two dimensions. If we take very heavy particles interacting with a light particle, in the extreme limit of *static* heavy particles one recovers the following model:

$$\begin{aligned} H \;=\; & \iint_{\mathbb{R}^2} \frac{d^2\mathbf{p}}{(2\pi)^2}\,\sqrt{\left(\mathbf{p}^2+m^2\right)}\; a^\dagger(\mathbf{p})a(\mathbf{p}) \\ & - \sum_{i=1}^N \lambda_i \phi^{(-)}(\mathbf{a_i})\phi^{(+)}(\mathbf{a_i})\,, \end{aligned} \tag{45}$$

where $\mathbf{a_i}$ refer to the locations of static heavy particles. Here

$$\begin{aligned} \phi^{(+)}(\mathbf{x}) \;&=\; \iint_{\mathbb{R}^2} \frac{d^2\mathbf{p}}{(2\pi)^2}\;\frac{e^{i\mathbf{p}\cdot\mathbf{x}}}{\sqrt{2}(\mathbf{p}^2+m^2)^{1/4}} a(\mathbf{p}) \quad \text{and} \\ \phi^{(-)} \;&=\; \left(\phi^{(+)}\right)^\dagger\,, \end{aligned} \tag{46}$$

where † denotes the adjoint. Since this model was worked out in Dogan and Turgut [17], we will be content with the resulting formulae only referring to the original paper for the details. We can compute the diagonal principal matrix as

$$\Phi_{ii}(z) = \frac{1}{2\pi}\ln\left(\frac{m-z}{m-E_B^i}\right)\,, \tag{47}$$

and the off-diagonal part as

$$\Phi_{ij}(z) = -\frac{1}{2\pi}\int_0^\infty \frac{ds}{(s^2+1)^{1/2}}\, e^{-|\mathbf{a_i}-\mathbf{a_j}|[m(s^2+1)^{1/2}-zs]}\,, \quad (48)$$

for $-m < \Re(z) < m$. Moreover, the binding energy of the single center should satisfy $-m < E_B^i < m$, and the lower bound is due to the stability requirement, to prevent pair creation to reduce the energy further thus rendering the model unrealistic in single particle sector.

2.5. Dirac Delta Interactions Supported by Curves in $\mathbb{R}^2$ and in $\mathbb{R}^3$

We consider N Dirac delta potentials supported by non-intersecting smooth curves $\gamma_\mathbf{j}:[0,L_j] \to \mathbb{R}^n$ of finite length L_j ($n = 2, 3$). Each curve is assumed to be simple, i.e., $\gamma_\mathbf{j}(s_1) \neq \gamma_\mathbf{j}(s_2)$ whenever $s_1 \neq s_2$, where $s_1, s_2 \in (0, L_j)$. Our formulation also allows the simple closed curves.

The Hamiltonian of the system is given by

$$H = H_0 - \sum_{i=1}^N \frac{\lambda_i}{L_i}|\gamma_\mathbf{i}\rangle\langle\gamma_\mathbf{i}|\,, \quad (49)$$

where $\langle\gamma_\mathbf{i}|\mathbf{r}\rangle = \int_{\Gamma_i} ds\ \delta(\mathbf{r}-\gamma_\mathbf{i}(s))$. Then, the Schrödinger equation ($H|\psi\rangle = E|\psi\rangle$) associated with this Hamiltonian is

$$-\nabla^2\psi(\mathbf{r}) - \sum_{i=1}^N \frac{\lambda_i}{L_i}\int_{\Gamma_i} ds_i\ \delta(\mathbf{r}-\gamma_\mathbf{i}(s_i))\int_{\Gamma_i} ds_i'\ \psi(\gamma_\mathbf{i}(s_i')) = E\psi(\mathbf{r})\,. \quad (50)$$

In contrast to the point-like Dirac delta interactions, this equation is a generalized Schrödinger equation in the sense that it is non-local. The resolvent kernel of the above Hamiltonian is explicitly given in the same form associated with point like Dirac delta potentials, namely

$$R(\mathbf{r_1},\mathbf{r_2};z) = R_0(\mathbf{r_1},\mathbf{r_2};z) + \sum_{i,j=1}^N \frac{1}{\sqrt{L_iL_j}} R_0(\mathbf{r_1},\gamma_\mathbf{i};z)\left[\Phi(z)\right]^{-1}_{ij} R_0\left(\gamma_\mathbf{j},\mathbf{r_2};z\right), \quad (51)$$

where

$$\Phi_{ij}(z) = \begin{cases} \frac{1}{\lambda_i} - \frac{1}{L_i}\langle\gamma_\mathbf{i}|R_0(z)|\gamma_\mathbf{i}\rangle & \text{if } i=j \\ -\frac{1}{\sqrt{L_iL_j}}\langle\gamma_\mathbf{i}|R_0(z)|\gamma_\mathbf{j}\rangle & \text{if } i\neq j \end{cases}, \quad (52)$$

or if we express it in terms of the heat kernel

$$\Phi_{ij}(z) = \begin{cases} \frac{1}{\lambda_i} - \frac{1}{L_i}\iint_{\Gamma_i\times\Gamma_i} ds_i\ ds_i'\ \int_0^\infty dt\ e^{tz}\ K_t(\gamma_\mathbf{i}(s_i),\gamma_\mathbf{i}(s_i')) & \text{if } i=j \\ -\frac{1}{\sqrt{L_iL_j}}\iint_{\Gamma_i\times\Gamma_j} ds_i\ ds_j'\ \int_0^\infty dt\ e^{tz}\ K_t(\gamma_\mathbf{i}(s_j),\gamma_\mathbf{j}(s_j')) & \text{if } i\neq j \end{cases}. \quad (53)$$

Using the explicit form of the heat kernel in two dimensions, the above principal matrix becomes

$$\Phi_{ij}(z) = \begin{cases} \frac{1}{\lambda_i} - \frac{i}{8\pi L_i}\iint_{\Gamma_i\times\Gamma_i} ds_i\ ds_i'\ H_0^{(1)}(\sqrt{z}|\gamma_\mathbf{i}(s_i)-\gamma_\mathbf{i}(s_i')|) & \text{if } i=j \\ -\frac{i}{8\pi\sqrt{L_iL_j}}\iint_{\Gamma_i\times\Gamma_j} ds_i\ ds_j'\ H_0^{(1)}(\sqrt{z}|\gamma_\mathbf{i}(s_i)-\gamma_\mathbf{j}(s_j')|) & \text{if } i\neq j \end{cases}. \quad (54)$$

The spectrum of the free Hamiltonian includes only continuous spectrum starting from zero, so we expect that the bound state energies must be below $z = 0$. For this reason, we restrict the principal matrix to the negative real values, i.e., $z = -\nu^2$, $\nu > 0$. Then, we have

$$\Phi_{ij}(z)|_{z=-\nu^2} = \begin{cases} \frac{1}{\lambda_i} - \frac{1}{4\pi L_i}\iint_{\Gamma_i\times\Gamma_i} ds_i\ ds_i'\ K_0(\nu|\gamma_\mathbf{i}(s_i)-\gamma_\mathbf{i}(s_i')|) & \text{if } i=j \\ -\frac{1}{4\pi\sqrt{L_iL_j}}\iint_{\Gamma_i\times\Gamma_j} ds_i\ ds_j'\ K_0(\nu|\gamma_\mathbf{i}(s_i)-\gamma_\mathbf{j}(s_j')|) & \text{if } i\neq j \end{cases}. \quad (55)$$

For non self-intersecting curve γ_i, we can expand it around the neighborhood of $s_i' = s_i$ in the Serret-Frenet frame at s_i [33]:

$$\gamma_\mathbf{i}(s_i') = \gamma_\mathbf{i}(s_i) + \left((s_i'-s_i) - k_i^2(s_i)\frac{(s_i'-s_i)^3}{3!}\right)\mathbf{t}_i(s_i) + \left(\frac{k_i(s_i)}{2}(s_i'-s_i)^2 - k_i'(s_i)\frac{(s_i'-s_i)^3}{3!}\right)\mathbf{n}_i(s_i) + \mathbf{R}_i(s_i)\,, \quad (56)$$

where $\mathbf{t}_i(s_i)$ and $\mathbf{n}_i(s_i)$ are the tangent and normal vectors at s_i, and $\mathbf{R}_i(s_i)$ is the remainder term which vanishes faster than $(s_i'-s_i)^3$ as $s_i' \to s_i$. We have an extra term proportional to the binormal vector $\mathbf{b}_i(s_i)$ in three dimensions ($-\frac{k_i(s_i)\tau_i(s_i)}{3!}(s_i'-s_i)^3\mathbf{b}_i(s_i)$, where $\tau_i(s_i)$ is the torsion of the curve). In the first approximation, keeping only the linear terms in $s_i'-s_i$, and translating and rotating the Serret-Frenet frame attached to the coordinate system Oxy in such a way that $\mathbf{t}_i(s_i) = (1,0)$ and $\mathbf{n}_i(s_i) = (0,1)$, we have

$$|\gamma_\mathbf{i}(s_i') - \gamma_i(s_i)| \approx |s_i'-s_i|\,. \quad (57)$$

Then, the integral in the diagonal part of the principal matrix (55) around $s_i' = s_i$ in the first approximation is

$$\iint_{\Gamma_i\times\Gamma_i} ds_i\ ds_i'\ K_0(\nu|s_i'-s_i|)\,. \quad (58)$$

By making change of coordinates $\xi_i = \frac{(s_i'+s_i)}{2}$ and $\eta_i = \frac{(s_i'-s_i)}{2}$, the above integral becomes

$$4\int_0^{L_i/2} d\eta_i(L_i-2\eta_i)K_0(2\nu\eta_i)\,. \quad (59)$$

Using $\int_0^{L_i/2} d\eta_i(L_i-2\eta_i)K_0(2\nu\eta_i) \leq \int_0^\infty d\eta_i(L_i-2\eta_i)K_0(2\nu\eta_i)$ and the integrals of modified Bessel functions [34]

$$\int_0^\infty dx\ x^n\,K_0(ax) = 2^{n-1}a^{-n-1}\Gamma^2\left(\frac{1+n}{2}\right), \quad (60)$$

where $n = 0, 1$ and Γ is the gamma function, it is easy to see that the integral that we consider is finite around $\eta_i = 0$ ($s_i' = s_i$). For non self-intersecting curves, the integrals in the diagonal and off-diagonal terms in (55) are finite whenever $s_i' \neq s_i$ due to the upper bounds of the Bessel functions [14]

$$K_0(x) < \frac{2}{1+x}e^{-\frac{x}{2}} + e^{-\frac{x}{2}}\ln\left(\frac{x+1}{x}\right). \quad (61)$$

In three dimensions, the Dirac delta potentials supported by curves requires the renormalization. Using the explicit formula of the heat kernel (23) for three dimensions, we find

$$\Phi_{ij}(z) = \begin{cases} \frac{1}{\lambda_i} - \frac{1}{4\pi L_i} \iint_{\Gamma_i\times\Gamma_i} ds_i\, ds_i' \, \frac{e^{i\sqrt{z}|\gamma_i(s_i)-\gamma_i(s_i')|}}{|\gamma_i(s_i)-\gamma_i(s_i')|} & \text{if } i=j \\ -\frac{1}{4\pi\sqrt{L_iL_j}} \iint_{\Gamma_i\times\Gamma_j} ds_i\, ds_j' \, \frac{e^{i\sqrt{z}|\gamma_i(s_i)-\gamma_j(s_j')|}}{|\gamma_i(s_i)-\gamma_j(s_j')|} & \text{if } i\neq j \end{cases} . \tag{62}$$

One can show that the diagonal part of the above principal matrix (53) includes a term

$$\iint_{\Gamma_i\times\Gamma_i} ds_i\, ds_i' \, \frac{e^{i\sqrt{z}|\gamma_i(s_i)-\gamma_i(s_i')|}}{|\gamma_i(s_i)-\gamma_i(s_i')|} , \tag{63}$$

which is divergent around $s_i' = s_i$. This can be immediately seen using the similar method outlined above, that is, the above integral includes the following integral in the new variable η_i:

$$\int_0^{L_i/2} d\eta_i \, \frac{e^{2i\sqrt{z}\eta_i}}{\eta_i} , \tag{64}$$

which is divergent around $\eta_i = 0$.

Similar to the non-relativistic and relativistic point interactions, we first regularize the resolvent and then by choosing the coupling constant as a function of the cut-off parameter ϵ:

$$\frac{1}{\lambda_i(\epsilon)} = \int_0^\infty dt\; e^{tE_B^i} K_{t+\epsilon}(\gamma_i(s_i),\gamma_i(s_i')) , \tag{65}$$

and taking the formal limit $\epsilon \to 0^+$, we obtain the resolvent which is exactly the same form as in (51) except the matrix Φ is given by

$$\Phi_{ij}(z) = \begin{cases} \frac{1}{L_i} \iint_{\Gamma_i\times\Gamma_i} ds_i\, ds_i' \int_0^\infty dt\, (e^{tE_B^i} - e^{tz}) K_t(\gamma_i(s_i),\gamma_i(s_i')) & \text{if } i=j \\ -\frac{1}{\sqrt{L_iL_j}} \iint_{\Gamma_i\times\Gamma_j} ds_i\, ds_j' \int_0^\infty dt\, e^{tz}\, K_t(\gamma_i(s_i),\gamma_j(s_j')) & \text{if } i\neq j \end{cases} . \tag{66}$$

Here, E_B^i is the bound state energy of the particle to the delta interaction supported by ith curve in the absence of all the other delta interactions. Since the spectrum of the free Hamiltonian only includes the continuous part starting from zero, we have $E_B^i < 0$. Using the explicit form of the heat kernel, the principal matrix turns out to be a finite expression:

$$\Phi_{ij}(z) = \begin{cases} \frac{1}{4\pi L_i} \iint_{\Gamma_i\times\Gamma_i} ds_i\, ds_i' \, \frac{1}{|(\gamma_i(s_i)-\gamma_i(s_i'))|} (e^{-\sqrt{|E_B^i|}|(\gamma_i(s_i)-\gamma_i(s_i'))|} - e^{i\sqrt{z}|(\gamma_i(s_i)-\gamma_i(s_i'))|}) & \text{if } i=j \\ -\frac{1}{4\pi\sqrt{L_iL_j}} \iint_{\Gamma_i\times\Gamma_j} ds_i\, ds_j' \, \frac{e^{i\sqrt{z}|(\gamma_i(s_i)-\gamma_j(s_j'))|}}{|(\gamma_i(s_i)-\gamma_j(s_j'))|} & \text{if } i\neq j \end{cases} . \tag{67}$$

A semi-relativistic generalization of particles interacting with curves is presented in Kaynak and Turgut[19]. The formal Hamiltonian can be written as

$$H = \iint_{\mathbb{R}^2} \frac{d^2\mathbf{p}}{(2\pi)^2} \left(\mathbf{p}^2 + m^2\right) a^\dagger(\mathbf{p}) a(\mathbf{p}) - \sum_{i=1}^N \frac{\lambda_i}{L_i} \int ds_i\, \phi^{(-)}(\gamma_i(s_i)) \int ds_i'\, \phi^{(+)}(\gamma_i(s_i')). \tag{68}$$

We refer to this work for the details and we are content with writing down the resulting Φ matrix, since for tunneling corrections to the bound spectra this is all we need:

$$\Phi_{ii}(z) = \frac{m}{\sqrt{2}\pi^2 L_i} \int_0^\infty dt \int_{\Gamma_i\times\Gamma_i} ds_i ds_i' \, \frac{K_1\left(m\sqrt{t^2+|\gamma_i(s_i)-\gamma_i(s_i')|^2}\right)}{\sqrt{t^2+|\gamma_i(s_i)-\gamma_i(s_i')|^2}} \left(e^{E_B^i t} - e^{zt}\right), \tag{69}$$

$$\Phi_{ij}(z) = -\frac{m}{\sqrt{2L_iL_j}\pi^2} \int_0^\infty dt \int_{\Gamma_i\times\Gamma_j} ds_i ds_j \, \frac{K_1\left(m\sqrt{t^2+|\gamma_i(s_i)-\gamma_j(s_j)|^2}\right)}{\sqrt{t^2+|\gamma_i(s_i)-\gamma_j(s_j)|^2}} e^{zt} . \tag{70}$$

As usual, these formulae must be analytically continued in z outside of their region of convergence. In our approach we are interested in the bound states for which these formulae are valid.

3. ANALYTIC STRUCTURE OF THE PRINCIPAL MATRICES AND THE BOUND STATE SPECTRUM

It is well-known that the bound state spectrum is determined by the poles of the resolvent, so the bound state spectrum should only come from the points z below the spectrum of the free Hamiltonian, where the matrix Φ is not invertible, i.e., the bound state energies are the real solutions of the equation

$$\det \Phi(E) = 0 , \tag{71}$$

where $E < \sigma(H_0)$. From all the explicit form of the principal matrices $\Phi_{ij}(z)$, they are all matrix-valued holomorphic function on their largest possible set of the complex plane. The analytical structure of the principal matrices can be determined by using the generalized Loewner's theorem [35], which simply states that if f_0 is a real valued continuously differentiable function on an open subset Δ of $(-\infty,\infty)$, then the following are equivalent:

- There exists a holomorphic function f with $\Im f \geq 0$ on the upper half-plane of the complex plane such that f has an analytic continuation across Δ that coincides with f_0 on Δ.
- For each continuous complex valued function F on Δ that vanishes off a compact subset of Δ,

$$\int_\Delta \int_\Delta d\zeta\; d\eta\; K(\zeta,\eta)\bar{F}(\zeta)F(\eta) \geq 0 , \tag{72}$$

where for $\zeta,\eta \in \Delta$,

$$K(\zeta,\eta) = \begin{cases} \frac{f_0(\zeta)-f_0(\eta)}{\zeta-\eta} & \text{if } \zeta\neq\eta \\ f_0'(\zeta) & \text{if } \zeta=\eta \end{cases} . \tag{73}$$

For simplicity, let us explicitly show the analytical structure of the principal matrix associated with the Dirac delta potential supported by a single curve in two dimensions. In this case, the principal matrix (52) is just the diagonal part, say $\Phi(E)$, and continuously differentiable function of E, where E is on the negative real axis. Then, we have

$$\frac{\Phi(\zeta)-\Phi(\eta)}{\zeta-\eta}=-\frac{1}{L}\frac{1}{\zeta-\eta}\langle\gamma|R_0(\zeta)-R_0(\eta)|\gamma\rangle\,, \tag{74}$$

where ζ,η is on the negative real axis and L is the length of the curve Γ. Using the resolvent identity for the free resolvent, i.e., $R_0(\zeta)-R_0(\eta)=(\eta-\zeta)R_0(\zeta)R_0(\eta)$, we find

$$\begin{aligned}&\int_\Delta\int_\Delta d\zeta\; d\eta\;\bar{F}(\zeta)F(\eta)\left(\frac{\Phi(\zeta)-\Phi(\eta)}{\zeta-\eta}\right)\\&=\frac{1}{L}\left|\int_\Delta d\eta\;F(\eta)R_0(\eta)|\gamma\rangle\right|^2>0\,,\end{aligned} \tag{75}$$

where $R_0^\dagger(\eta)=R_0(\bar{\eta})=R_0(\eta)$. The positivity is preserved in the limiting case $\zeta\to\eta$ as well. This shows that the analytically continued function, say $\tilde{\Phi}$ is a Nevallina function. We denote the analytically continued function by the same letter Φ for simplicity. The aforementioned theorem can be generalized to the matrix valued function $\Phi_{ij}(E)$, as a result to ensure the holomorphicity we verify that:

$$\begin{aligned}&\int_\Delta\int_\Delta d\zeta\; d\eta\;\sum_{i,j=1}^{N}\bar{F}_i(\zeta)F_j(\eta)\left(\frac{\Phi_{ij}(\zeta)-\Phi_{ij}(\eta)}{\zeta-\eta}\right)\\&=\left|\int_\Delta d\eta\;\sum_{i=1}^{N}\frac{1}{L_i}F_i(\eta)R_0(\eta)|\gamma_i\rangle\right|^2>0\,,\end{aligned} \tag{76}$$

and the principal matrix in all the other cases including the relativistic extension of the problem can be similarly analyzed. Hence, for a large region of the complex plane, which contains the negative real axis, the principal matrix is a matrix-valued holomorphic function so that its eigenvalues and eigenprojections are holomorphic near the real axis [36]. In fact, we get poles on the real axis for the eigenvalues and the residue calculus can be used the calculate the associated projections.

Let us consider the eigenvalue problem for the principal matrix depending on the real parameter E:

$$\Phi(E)A^k(E)=\omega^k(E)A^k(E)\,, \tag{77}$$

where $k=1,2,\ldots,N$ and we assume there is no degeneracy for simplicity (we consider the generic case). In order to simplify the notation, we sometimes suppress the variable E in the equations, e.g., $A^k(E)=A^k$ and so on. Then, the bound state energies can be found from the zeroes of the eigenvalues ω, that is,

$$\omega^k(E)=0\,, \tag{78}$$

for each k. Thanks to Feynman-Hellmann theorem [37, 38], we have the following useful result

$$\frac{\partial\omega^k}{\partial E}=\langle A^k,\frac{\partial\Phi}{\partial E}\,A^k\rangle\,, \tag{79}$$

where $\langle .,.\rangle$ denotes the inner product on $\mathbb{C}^N$. Using the expression of the principal matrices in all class of singular interactions described above and using the positivity of the heat kernel, it is possible to show that

$$\frac{\partial\omega^k}{\partial E}<0\,. \tag{80}$$

This is an important result, since it implies that every eigenvalue cuts the real axis only once, that particular value gives us a bound state if it is below the spectrum of the free part. Moreover, we deduce that the ground state energy corresponds to the smallest eigenvalue of Φ.

4. OFF-DIAGONAL TERMS OF THE PRINCIPAL MATRICES IN THE TUNNELING REGIME

For simplicity, we assume that all binding energies E_B^i's or/and λ_i's are different. We consider the situation where the Dirac delta potentials (supported by points and curves) are separated far away from each other in the sense that the de Broglie wavelength of the particle is much smaller than the minimum distance d between the point Dirac delta potentials or than the minimum distance between the delta potentials supported by non-intersecting regular curves with finite length, namely

$$d\gg\lambda_{\text{de Broglie}}\,, \tag{81}$$

or in the semi-relativistic case, this can be stated as $d\gg\lambda_{\text{Compton}}$. This regime can be also defined in terms of the energy scales, namely

$$\frac{1}{d^2}\ll E_B\,, \tag{82}$$

where E_B is the minimum of the binding energies to the single delta potentials in the absence of all the others (recall that $\hbar=2m=1$).

In the non-relativistic problem for point interactions in one and three dimensions, it is clear from the explicit form of the principal matrices (18), (33) all the off-diagonal terms are getting exponentially small as d increases, i.e.,

$$|\Phi_{ij}(\nu)|=\frac{\exp(-\nu d_{ij})}{2\nu}\leq\frac{\exp(-\nu d)}{2\nu}\to 0\,, \tag{83}$$

and

$$|\Phi_{ij}(\nu)|=\frac{\exp(-\nu d_{ij})}{4\pi\,d_{ij}}\leq\frac{\exp(-\nu d)}{4\pi\,d}\to 0\,, \tag{84}$$

as $d\to\infty$. For point interactions in two dimensions, thanks to the upper bound of the Bessel function [14],

$$K_0(x)<\frac{2}{x}\exp(-x/2)\,, \tag{85}$$

for all x, the off-diagonal terms of the principal matrix (32)

$$|\Phi_{ij}(\nu)| \leq \frac{1}{2\pi} K_0(\nu|\mathbf{a_i}-\mathbf{a_j}|) \leq \frac{1}{2\pi} K_0(\nu d) < \frac{1}{\nu\pi d}\exp(-\nu d)\,, \tag{86}$$

is going to zero exponentially as $d \to \infty$. In the above expressions for principal matrices, we have expressed them in terms of a real positive variable ν for simplicity. Not all the bound state spectrum of the potentials we consider in this paper is negative, so it is not always useful to express the principal matrix in terms of a real positive variable ν. For that purpose, we will consider the principal matrices restricted to the real values, namely $z = E$, where E is the real variable (not necessarily negative).

For point interactions in three dimensional hyperbolic manifolds, the off-diagonal principal matrix restricted to the real values $E < \kappa^2$

$$|\Phi_{ij}(E)| \leq \left(\frac{\kappa \exp\left(-d\sqrt{\kappa^2 - z}\right)}{4\pi \sinh\left(\kappa d\right)}\right) \tag{87}$$

is exponentially small as $d \to \infty$. Here d is the minimum geodesic distance between the centers.

As for the point interactions in two dimensional hyperbolic manifolds, the off-diagonal principal matrix restricted to the real values $E < \kappa^2/4$ becomes

$$|\Phi_{ij}(E)| = \frac{1}{2\pi}\, Q_{\frac{1}{2}+\sqrt{-\frac{E}{\kappa^2}+\frac{1}{4}}}\left(\cosh(\kappa d(a_i,a_j))\right)\,. \tag{88}$$

Using the series representation of the Legendre function of second kind [28]

$$Q_\nu(\cosh\alpha) = \sum_{k=0}^{\infty} \frac{\Gamma(k+\nu+1)\Gamma\left(k+\frac{1}{2}\right)}{\Gamma\left(k+\nu+\frac{3}{2}\right)\Gamma(k+1)} e^{-\alpha(2k+\nu+1)}\,, \tag{89}$$

where $\nu = \frac{1}{2} + \sqrt{-\frac{E}{\kappa^2}+\frac{1}{4}} > 1$ and $\alpha = \kappa d(a_i,a_j)$, and splitting the sum, we obtain

$$\begin{aligned} |\Phi_{ij}(E)| \;=\; & \frac{\Gamma(\nu+1)\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\nu+\frac{3}{2}\right)\Gamma(1)} e^{-\alpha(\nu+1)} \\ & + \frac{\Gamma(1+\nu+1)\Gamma\left(1+\frac{1}{2}\right)}{\Gamma\left(1+\nu+\frac{3}{2}\right)\Gamma(1+1)} e^{-\alpha(2+\nu+1)} \\ & + \sum_{k=2}^{\infty} \frac{\Gamma(k+\nu+1)\Gamma\left(k+\frac{1}{2}\right)}{\Gamma\left(k+\nu+\frac{3}{2}\right)\Gamma(k+1)} e^{-\alpha(2k+\nu+1)}\,. \end{aligned} \tag{90}$$

Since Gamma function is increasing on $[2,\infty]$, $\frac{\Gamma(k+\nu+1)\Gamma\left(k+\frac{1}{2}\right)}{\Gamma\left(k+\nu+\frac{3}{2}\right)\Gamma(k+1)} < 1$ for all $k \geq 2$, and $\nu > 1$, we can find an upper bound for the above the infinite sum as

$$e^{-4\kappa d-\kappa d(\nu+1)} \sum_{k=0}^{\infty} e^{-2k\kappa d}\,, \tag{91}$$

which is simply a geometric series. All these show that the off-diagonal principal matrix in two dimensional hyperbolic manifolds is exponentially small as $d \to \infty$ and the leading term is given by the first term of the series expansion.

As for the delta interactions supported by curves, the minimum of the pairwise distances between the supports of Dirac delta potentials always exists since $d_{ij}(s,s') = \sqrt{|(\gamma_\mathbf{i}(\mathbf{s}) - \gamma_\mathbf{j}(\mathbf{s}'))|}$ is a continuous function on compact interval $s \in [0,L]$, so we have

$$|(\gamma_\mathbf{i}(s_i) - \gamma_\mathbf{j}(s_j'))|^2 \geq \min_{s_i,s_j'} |(\gamma_\mathbf{i}(s_i) - \gamma_\mathbf{j}(s_j'))|^2 := d_{ij} \geq \min_{ij} d_{ij} := d\,, \tag{92}$$

for $i \neq j$. Then,

$$|\Phi_{ij}(E)| \leq \sqrt{L_i\, L_j} \int_0^\infty dt\, \frac{e^{-d^2/4t+tE}}{4\pi t} = \frac{\sqrt{L_i\, L_j}}{2\pi} K_0(\sqrt{-E}d)\,. \tag{93}$$

Due to the upper bound of the Bessel function (85), the off-diagonal principal matrix is going to zero as $d \to \infty$.

Similarly, the explicit forms of the off-diagonal parts of the principal matrices (44) and (48) in the relativistic cases are exponentially going to zero as $d \to \infty$ (by assuming the order of the limit and the integral can be interchanged). For the other relativistic cases (including the relativistic delta potentials supported by curves), the off diagonal terms of the principal matrices can also be shown to be exponentially small.

Therefore, we see that the principal matrices for all the above models are diagonally dominant in the "large" separation regime. However, the exponentially small off-diagonal terms are not analytic in the small parameter ($\frac{1}{E_B d^2}$). Nevertheless, we can keep track of small values of the off-diagonal terms by introducing an artificial parameter ϵ in order to control the orders of terms in the perturbative expansion, that we are going to develop in the next section.

5. SPLITTING IN BOUND STATE ENERGIES THROUGH PERTURBATION THEORY

Let us consider the family of principal matrices restricted to the real axis E:

$$\Phi(E) = \Phi_0(E) + \epsilon\, \delta\Phi(E)\,, \tag{94}$$

where Φ_0 is the diagonal part of the principal matrix, and $\delta\Phi$ is off-diagonal part of it and this is the "small" correction (perturbation) to the diagonal part. Since $\Phi(E)$ is symmetric (Hermitian), we can apply standard perturbation techniques to the principal matrix [5, 36, 39]. For this purpose, let us assume we can expand the eigenvalues and eigenvectors as follows:

$$\begin{aligned} \omega^k &= \omega_0^k + \epsilon\, \omega_1^k + \epsilon^2\, \omega_2^k + \dots \\ A^k &= A_0^k + \epsilon\, A_1^k + \epsilon^2\, A_2^k + \dots\,, \end{aligned} \tag{95}$$

for each k.

The solution to the related unperturbed eigenvalue problem

$$\Phi_0 A_0^k = \omega_0^k A_0^k\,, \tag{96}$$

is given by

$$\omega_0^k = [\Phi_0]_{kk} \,. \tag{97}$$

Once we have found the eigenvalues and eigenvectors of the diagonal part of the principal matrix or unperturbed eigenvalue problem, we can perturbatively solve the full problem. The standard perturbation theory gives us the eigenvalues ω^k up to second order:

$$\omega_1^k(E) \,=\, \langle A_0^k(E), \delta\Phi(E) A_0^k(E)\rangle = \left[\delta\Phi(E)\right]_{kk} \,, \tag{98}$$

$$\begin{aligned}\omega_2^k(E) \,&=\, \sum_{\substack{l=1\\ l\neq k}}^{N} \frac{\left|\langle A_0^k(E), \delta\Phi(E) A_0^k(E)\rangle\right|^2}{\omega_0^k(E) - \omega_0^l(E)} \\ &= \sum_{\substack{l=1\\ l\neq k}}^{N} \frac{\Phi_{lk}(E)\Phi_{kl}(E)}{\omega_0^k(E) - \omega_0^l(E)} \,.\end{aligned} \tag{99}$$

and the first order correction to the eigenvectors A^k is given by

$$A_1^k(E) = \sum_{\substack{j=1\\ j\neq k}}^{N} \frac{\delta\Phi_{jk}(E)}{\omega_0^k(E) - \omega_0^j(E)} \, A_0^j(E) \,. \tag{100}$$

Since the bound state energies are determined from the solution of Equation (78), the bound state energies in the zeroth order approximation can easily be found from $\omega_0^k(E) = 0$. The solution is given by

$$E = E_0^k = E_B^k \,, \tag{101}$$

and the corresponding eigenvector is

$$A_0^k(E_B^k) \equiv A_0^k \equiv \mathbf{e}^k \equiv \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} \,, \tag{102}$$

where 1 is located in the kth position of the column and other elements of it are zero or we can write

$$A_0^{ki} = e_i^k = \delta_{ki} \,. \tag{103}$$

Here e_i^k s form a complete orthonormal set of basis.

$$\sum_{i=1}^{N} e_i^k e_i^l = \delta_{kl} \,. \tag{104}$$

The bound state energies to the full problem up to the second order is then determined by solving the following equation

$$\omega^k(E) = \omega_0^k(E) + \epsilon^2 \, \omega_2^k(E) = 0 \,, \tag{105}$$

where we have used the first order result

$$\omega_1^k = 0 \tag{106}$$

from the Equation (98).

Let us now expand $\omega_0^k(E)$ and $\Phi_{kl}(E)$ for $k \neq l$ around $E = E_B^k$:

$$\begin{aligned}\omega_0^k(E) \,&=\, \left.\frac{\partial\omega_0^k(E)}{\partial E}\right|_{E=E_B^k} \delta E^k + \mathcal{O}((\delta E^k)^2) \,, \\ \Phi_{kl}(E) \,&=\, \Phi_{kl}(E_B^k) + \left.\frac{\partial\Phi_{kl}(E)}{\partial E}\right|_{E=E_B^k} \delta E^k + \mathcal{O}((\delta E^k)^2) \,,\end{aligned} \tag{107}$$

where $\omega_0^k(E_B^k) \,=\, 0$. If we substitute (107) into (105) and (99), and use Feynman-Hellman theorem given in previous section, the condition (105) up to the second order turns out be

$$\begin{aligned}&\left.\frac{\partial\Phi_{kk}(E)}{\partial E}\right|_{E=E_B^k} \delta E^k - \epsilon^2 \sum_{\substack{l=1\\ l\neq k}}^{N} \frac{1}{\Phi_{ll}(E_B^k)} \Bigg[\Phi_{kl}(E_B^k)\Phi_{lk}(E_B^k) \\ &+ \left(\Phi_{kl}(E_B^k) \left.\frac{\partial\Phi_{lk}(E)}{\partial E}\right|_{E=E_B^k} + \Phi_{lk}(E_B^k) \left.\frac{\partial\Phi_{kl}(E)}{\partial E}\right|_{E=E_B^k} \right)\delta E^k \Bigg] \\ &\times \left[1 + \frac{1}{\Phi_{ll}(E_B^k)} \left(\left.\frac{\partial\Phi_{ll}(E)}{\partial E}\right|_{E=E_B^k} - \left.\frac{\partial\Phi_{kk}(E)}{\partial E}\right|_{E=E_B^k} \right)\delta E^k \right]^{-1} \\ &+ \mathcal{O}((\delta E^k)^2) = 0 \,.\end{aligned} \tag{108}$$

If we also expand the last factor in the powers of (δE^k) and ignore the second order terms and combine the terms using the symmetry property of principal matrix, we find

$$\begin{aligned}&\left[\left.\frac{\partial\Phi_{kk}(E)}{\partial E}\right|_{E=E_B^k} + \epsilon^2 \sum_{\substack{l=1\\ l\neq k}}^{N} \frac{\Phi_{kl}(E_B^k)\Phi_{lk}(E_B^k)}{\Phi_{ll}^2(E_B^k)} \left(\left.\frac{\partial\Phi_{ll}(E)}{\partial E}\right|_{E=E_B^k} \right.\right. \\ &\left.\left. - \left.\frac{\partial\Phi_{kk}(E)}{\partial E}\right|_{E=E_B^k} \right) - 2 \sum_{\substack{l=1\\ l\neq k}}^{N} \frac{\Phi_{kl}(E_B^k)}{\Phi_{ll}(E_B^k)} \left.\frac{\partial\Phi_{lk}(E)}{\partial E}\right|_{E=E_B^k} \right]\delta E^k \\ &= \epsilon^2 \sum_{\substack{l=1\\ l\neq k}}^{N} \frac{\Phi_{kl}(E_B^k)\Phi_{lk}(E_B^k)}{\Phi_{ll}(E_B^k)} + \mathcal{O}((\delta E^k)^2) \,.\end{aligned} \tag{109}$$

Ignoring the second and third terms on the left hand side of the equality (this is guaranteed by the assumption $\Phi_{kk}(E_B^k) \gg |\Phi_{kl}(E_B^k)|$) and setting $\epsilon \,=\, 1$, we get the change in E^k (to first order) as,

$$\delta E^k \simeq \left(\left.\frac{\partial\Phi_{kk}(E)}{\partial E}\right|_{E=E_B^k} \right)^{-1} \sum_{\substack{l=1\\ l\neq k}}^{N} \frac{\Phi_{kl}(E_B^k)\Phi_{lk}(E_B^k)}{\Phi_{ll}(E_B^k)} + \mathcal{O}((\delta E^k)^2) \,. \tag{110}$$

This is our main formula for all types of singular interactions we consider. It is striking that it contains the information about the tunneling regime.

6. EXPLICIT EXAMPLES FOR THE SPLITTING IN THE ENERGY

Let us now compute explicitly how the bound state energies change in the tunneling regime for the above class of singular potentials.

For point Dirac delta potentials in one dimension, the bound state energies are negative so $E_B^k = -|E_B^k|$ and

$$\delta E^k \simeq \sqrt{|E_B^k|} \sum_{\substack{l=1 \\ l\neq k}}^{N} \frac{1}{\left(\frac{1}{\lambda_l} - \frac{1}{2\sqrt{|E_B^k|}}\right)} \exp\left(-2\sqrt{|E_B^k|}\,|a_k - a_l|\right), \quad (111)$$

in the tunneling regime $d\sqrt{|E_B|} \gg 1$.

For point Dirac delta potentials in two dimensions, the bound state energies are negative and

$$\delta E^k \simeq \sum_{\substack{l=1 \\ l\neq k}}^{N} \frac{2\pi}{\sqrt{|E_B^k|}|\mathbf{a_k} - \mathbf{a_l}| \log(E_B^k/E_B^l)} \exp\left(-2\sqrt{|E_B^k|}|\mathbf{a_k} - \mathbf{a_l}|\right), \quad (112)$$

again in the tunneling regime. Here we have used the asymptotic expansion of the modified Bessel function of the third kind $K_0(x) \approx \sqrt{\frac{\pi}{2x}}\,\exp(-x)$ for $x \gg 1$ [28].

In three dimensions, we have

$$\delta E^k \simeq \sum_{\substack{l=1 \\ l\neq k}}^{N} \frac{2\sqrt{|E_B^k|}}{4\pi^2|\mathbf{a_k} - \mathbf{a_l}|^2} \frac{\exp\left(-2\sqrt{|E_B^k|}|\mathbf{a_k} - \mathbf{a_l}|\right)}{\left(\sqrt{|E_B^k|} - \sqrt{|E_B^l|}\right)}. \quad (113)$$

For point interactions in three dimensional hyperbolic manifolds, the bound state energies are below κ^2 (see [15] for details) and

$$\delta E^k \simeq \sqrt{\kappa^2 - E_B^k} \sum_{\substack{l=1 \\ l\neq k}}^{N} \frac{4\kappa^2}{\sqrt{\kappa^2 - E_B^k} - \sqrt{\kappa^2 - E_B^l}} \exp\left(-2d(a_k, a_l)\left(\kappa + \sqrt{\kappa^2 - E_B^k}\right)\right), \quad (114)$$

in the tunneling regime. Here we have used $\sinh^2 x \approx \frac{e^{2x}}{4}$ as $x \gg 1$.

For point interactions in two dimensional hyperbolic manifolds, the bound state energies are below $\kappa^2/4$ (see [15]) and

$$\delta E^k \simeq \frac{2\kappa^2\sqrt{\frac{1}{4} - \frac{E_B^k}{\kappa^2}}}{\psi^{(1)}\left(\frac{1}{2} + \sqrt{\frac{1}{4} - \frac{E_B^k}{\kappa^2}}\right)} \sum_{\substack{l=1 \\ l\neq k}}^{N} \frac{1}{\psi\left(\frac{1}{2} + \sqrt{\frac{1}{4} - \frac{E_B^k}{\kappa^2}}\right) - \psi\left(\frac{1}{2} + \sqrt{\frac{1}{4} - \frac{E_B^l}{\kappa^2}}\right)} \times \sum_{m=0}^{\infty} \frac{\Gamma\left(m + \frac{3}{2} + \sqrt{\frac{1}{4} - \frac{E_B^k}{\kappa^2}}\right)\Gamma(m + \frac{1}{2})}{\Gamma\left(m + 2 + \sqrt{\frac{1}{4} - \frac{E_B^k}{\kappa^2}}\right)\Gamma(m+1)} \exp\left(-\kappa\, d(a_k, a_l)\left(2m + \frac{3}{2} + \sqrt{\frac{1}{4} - \frac{E_B^k}{\kappa^2}}\right)\right), \quad (115)$$

where $\psi^{(1)}$ is the polygamma function and we have used the infinite series representation of the Legendre function of second kind (89).

For semi-relativistic point interactions in one dimensions, the bound state energies are below m. Let us first find explicitly integrals in the off-diagonal part of the principal matrix asymptotically

$$\frac{1}{\pi}\int_m^\infty d\mu e^{-\mu|a_k - a_l|} \frac{\sqrt{\mu^2 - m^2}}{\mu^2 - m^2 + (E_B^k)^2} \quad (116)$$

in the tunneling regime $md \gg 1$. For this purpose, let us rescale the integration variable $s = \mu/m$ so that the above integral becomes $\frac{m^2}{\pi}\int_1^\infty \frac{e^{-sm|a_k - a_l|}\sqrt{s^2-1}}{m^2(s^2-1)+(E_B^k)^2}$. Note that $-s$ in the exponent has its maximum at $s = 1$ on the interval $(1, \infty)$. Then, only the vicinity of $s = 1$ contributes to the full asymptotic expansion of the integral for large $m|a_k - a_l|$. Thus, we may approximate the above integral by $\frac{m^2}{\pi}\int_1^\epsilon \frac{e^{-sm|a_k - a_l|}\sqrt{s^2-1}}{m^2(s^2-1)+(E_B^k)^2}$, where $\epsilon > 1$ and replace the function $\frac{\sqrt{s^2-1}}{m^2(s^2-1)+(E_B^k)^2}$ in the integrand by its Taylor expansion [40]. It is important to emphasize that the full asymptotic expansion of this integral as $m|a_k - a_l| \to \infty$ does not depend on ϵ since all other integrations are subdominant compared to the original integral. Hence, we find

$$\begin{aligned} \frac{m^2}{\pi}\int_1^\epsilon \frac{e^{-sm|a_k - a_l|}\sqrt{s^2-1}}{m^2(s^2-1)+(E_B^k)^2} &\sim \frac{m^2}{\pi}\int_1^\epsilon ds\, e^{-sm|a_k - a_l|} \frac{\sqrt{2}\sqrt{s-1}}{(E_B^k)^2} \\ &\sim \frac{m^2}{\pi}\int_1^\infty ds\, e^{-sm|a_k - a_l|} \frac{\sqrt{2}\sqrt{s-1}}{(E_B^k)^2} \\ &\sim \frac{1}{\sqrt{2\pi}}\left(\frac{m}{E_B^k}\right)^2 \frac{1}{m|a_k - a_l|^{3/2}} \\ &\exp\left(-m|a_k - a_l|\right), \end{aligned} \quad (117)$$

where we have used the fact that the contribution to the integral outside of the interval $(1, \epsilon)$ is exponentially small. Substituting this result into Equation (110), we find

$$\delta E^k \simeq \left(\varphi'(E_B^k)\right)^{-1} \sum_{\substack{l=1 \\ l\neq k}}^{N} \frac{1}{2\pi}\left(\frac{m}{E_B^k}\right)^4 \frac{1}{m|a_k - a_l|^3} \frac{1}{\varphi(E_B^k) - \varphi(E_B^l)} \exp\left(-2m|a_k - a_l|\right) \quad (118)$$

when $E_B^k < 0$ and

$$\delta E^k \simeq \left(\varphi'(E_B^k)\right)^{-1} \sum_{\substack{l=1\\ l\neq k}}^{N} \frac{1}{\varphi(E_B^k)-\varphi(E_B^l)} \Bigg(\frac{e^{-\sqrt{m^2-(E_B^k)^2}|a_k-a_l|} E_B^k}{\sqrt{m^2-(E_B^k)^2}} + \frac{1}{\sqrt{2\pi}} \left(\frac{m}{E_B^k}\right)^2 \frac{1}{m|a_k-a_l|^{3/2}} \exp\left(-m|a_k-a_l|\right) \Bigg)^2 \tag{119}$$

when $E_B^k > 0$.

For the field theory motivated relativistic version we can use a saddle point approximation, assuming that tunneling condition, given by $\sqrt{m^2-(E_B^i)^2}d_{ij} >> 1$ is satisfied. Here it is enough to consider the function $m(1+s^2)^{1/2} - E_B^i s$ and expand it around the maximum $E_B^i/\sqrt{m^2-(E_B^i)^2}$. The denominator can be replaced by its value at the maximum, we find that the leading behavior goes as

$$\Phi_{ij}(E_B^i) \sim -\frac{1}{2\pi} \frac{\sqrt{m^2-(E_B^i)^2}}{m} e^{-d_{ij}\sqrt{m^2-(E_B^i)^2}} \int_{-E_B^i/\sqrt{m^2-(E_B^i)^2}}^{\infty} d\xi \; e^{-d_{ij}[m^2-(E_B^i)^2]^{3/2}\frac{\xi^2}{2m^2}}, \tag{120}$$

(assuming that $E_B^i d_{ij}$'s remain large) evaluating the integral we end up with,

$$\Phi_{ij} \sim -\frac{1}{\sqrt{2\pi}} \frac{1}{[d_{ij}\sqrt{m^2-(E_B^i)^2}]^{1/2}} e^{-d_{ij}\sqrt{m^2-(E_B^i)^2}}. \tag{121}$$

Once we obtain the off-diagonal terms responsible for the tunneling contributions, calculating the derivatives of the diagonal parts are simple,

$$\frac{\partial \Phi_{ii}(E)}{\partial E}\Big|_{E=E_B^i} = -\frac{1}{2\pi}\frac{1}{m-E_B^i}. \tag{122}$$

Substituting these expressions into the general formulae we have derived, will give the tunneling contribution to energy levels that leads to small shifts in the binding energies.

For Dirac delta potentials supported by curves in two dimensions: we define a kind of center of mass by

$$\mathbf{x}_i = \frac{1}{L_i}\int_{\Gamma_i} ds_i \, \gamma(s_i) \, , \tag{123}$$

and write

$$|\gamma(s_i)-\gamma_j(s_j)| = |\gamma(s_i)-\mathbf{x}_i-\gamma_j(s_j)+\mathbf{x}_j+(\mathbf{x}_i-\mathbf{x}_j)| \, , \tag{124}$$

in the argument of the functions in the principal matrix. When we evaluate the expressions we expand these terms by keeping only first order terms in the small quantities. The resulting Bessel functions can be expanded again to find the leading corrections for the curve to curve interaction terms. We use the expression above for the off diagonal terms and define $d_{ij} = |\mathbf{x}_i - \mathbf{x}_j|$ for simplicity and introduce a unit vector as $\hat{\mathbf{d}}_{\mathbf{ij}}$ in a similar way. As a result we have the leading order expansion,

$$K_0(\sqrt{-E}d_{ij}) - K_1(\sqrt{-E}d_{ij})\frac{1}{d_{ij}}\left[\hat{\mathbf{d}}_{\mathbf{ij}}\cdot(\gamma_i(s_i)-\mathbf{x}_i) - \hat{\mathbf{d}}_{\mathbf{ij}}\cdot(\gamma_j(s_j)-\mathbf{x}_j)\right]. \tag{125}$$

When we insert this into Φ_{ij} expression and integrate over the curve, we find

$$\int ds_i \, \hat{\mathbf{d}}_{\mathbf{ij}} \cdot (\gamma_i(s_i)-\mathbf{x}_i) = \hat{\mathbf{d}}_{\mathbf{ij}} \cdot \int ds_i \, (\gamma_i(s_i)-\mathbf{x}_i) = 0 \, , \tag{126}$$

and similarly for the other part. Thus, we see that the only contribution comes from the second order which we neglect for our purposes. However, a systematic expansion in powers of $\frac{1}{d_{ij}}$ can be developed for higher order correction as described. Using the asymptotic expansion of $K_0(z)$ for large values of z [28],

$$K_\nu(z) \sim \sqrt{\frac{\pi}{2z}} e^{-z}, \tag{127}$$

for all $\nu \geq 0$ we get from (110) a more elegant expression,

$$\delta E^k \simeq \left(\frac{\partial \Phi_{kk}(E)}{\partial E}\Big|_{E=E_B^k}\right)^{-1} \sum_{\substack{l=1\\ l\neq k}}^{N} \frac{\left(L_k L_l/8\pi\sqrt{|E_B^k|}d_{kl}\right)}{\left(\Phi_{ll}(E_B^k)\right)} \exp\left(-2\sqrt{|E_B^k|}d_{kl}\right) + \mathcal{O}((\delta E^k)^2) \, , \tag{128}$$

where Φ_{ll} and its derivative at E_B^k can be computed from the explicit expression of the principal matrix (54). For Dirac delta potentials supported by curves in three dimensions, there is really no change, since renormalization is required only for the diagonal parts, we have the off-diagonal expressions already in a simpler form, as a result of the above analysis, the leading order expression is found to be,

$$\delta E^k \simeq \left(\frac{\partial \Phi_{kk}(E)}{\partial E}\Big|_{E=E_B^k}\right)^{-1} \sum_{\substack{l=1\\ l\neq k}}^{N} \frac{\left(L_k L_l/16\pi^2 d_{kl}^2\right)}{\left(\Phi_{ll}(E_B^k)\right)} \exp\left(-2\sqrt{|E_B^k|}d_{kl}\right) + \mathcal{O}((\delta E^k)^2) \, , \tag{129}$$

where Φ_{ll} and its derivative at E_B^k can be computed from the explicit expression of the principal matrix (67).

In a similar way, we look at the tunneling correction to bound state energies for relativistic particle coupled to Dirac potentials supported over curves. Again we use the approximation that the separation of the curves are large and the extend of the curves compared to these distances are small. This is not the only possible approximation, one can envisage a situation in which the separations are large but the extend of the curves are also large.

The essential ideas are captured by our example so to achieve technical simplicity we keep this approximation. Essential point is to expand the off-diagonal terms in the leading order. By scaling t variable in the integral we can write $\Phi_{ij}(E_B^i)$ term as,

$$\begin{aligned}\Phi_{ij}(E_B^i) &= -\frac{m}{\sqrt{2L_iL_j}\pi^2}\int_0^\infty dt\int_{\Gamma_i\times\Gamma_j} ds_i ds_j\ \frac{K_1\big(m|\gamma(s_i)-\gamma(s_j)|\sqrt{t^2+1}\big)}{\sqrt{t^2+1}}e^{E_B^i t|\gamma(s_i)-\gamma(s_j)|}\\ &\sim -\int_{\Gamma_i\times\Gamma_j} ds_i ds_j\ \frac{m^{1/2}}{2\sqrt{|\gamma(s_i)-\gamma(s_j)|}(L_iL_j)^{1/2}\pi^{3/2}}\int_0^\infty dt\ \frac{e^{-|\gamma(s_i)-\gamma(s_j)|[m\sqrt{t^2+1}-E_B^i t]}}{(t^2+1)^{3/4}},\end{aligned} \tag{130}$$

where in the second line we used the asymptotics of K_1 for large argument (127). We may now use the same argument by means of the center of mass of the curves to define center to center distances and expand around the center of mass, not surprisingly we again find that the first order corrections become zero, only the center to center distance matters. Therefore, to leading order we have a simpler expression,

$$\Phi_{ij}(E_B^i) \sim -\frac{m^{1/2}(L_iL_j)^{1/2}}{2\pi^{3/2}d_{ij}^{1/2}}\int_0^\infty dt\ \frac{e^{-d_{ij}[m\sqrt{t^2+1}-E_B^i t]}}{(t^2+1)^{3/4}}. \tag{131}$$

This is of the type we have worked out for the semi-relativistic particle, and in the same manner, a saddle point approximation can be applied in a simple way, resulting

$$\Phi_{ij}(E_B^i) \sim -\frac{(L_iL_j)^{1/2}}{\sqrt{2}\pi\, d_{ij}}\ e^{-d_{ij}\sqrt{m^2-(E_B^i)^2}}\ . \tag{132}$$

We may now employ our general expressions to find the tunneling corrections. The derivative of the diagonal term can be simplified by means of $\frac{\partial K_0(z)}{\partial z} = -K_1(z)$.

7. DEGENERATE CASE AND WAVE FUNCTIONS FOR POINT INTERACTIONS

Let us now compute the energy splitting of two equal strength delta functions supported by the points $-\mathbf{a}$ and $\mathbf{a}$ in two dimensions. This is exactly the problem we discuss in the introduction, yet this version can be solved exactly. The approximation we use corresponds to the standard WKB approach. Let us recall that when we have two degenerate eigenvalues

$$\omega_0^1(E) = \omega_0^2(E), \tag{133}$$

the degeneracy is lifted by the diagonal perturbation and as is well-known the diagonalizing the perturbation matrix in the degeneracy subspace gives us the first order correction:

$$\begin{aligned}\omega_1^1(E) &= +|\Phi_{12}(E)|\ ,\\ \omega_1^2(E) &= -|\Phi_{12}(E)|\ .\end{aligned} \tag{134}$$

If we call the common bound state as E_B, for $k = 1, 2$ to get the first order correction we truncate the eigenvalue equations as,

$$\omega_0^k(E_B + E_1^k) + \omega_1^k(E_B) = 0 \tag{135}$$

which leads to

$$E_1^k \sim (-1)^{k+1}2|E_B|K_0(2\sqrt{|E_B|}a) \sim (-1)^{k+1}\frac{|E_B|^{3/4}\sqrt{\pi}}{\sqrt{a}}\ e^{-2\sqrt{|E_B|}a}\ , \tag{136}$$

where we have used the asymptotic expansion of K_0 given by (127). Thus, the splitting is given by

$$\delta E_1 = E_1^1 - E_1^2 \sim 2\frac{|E_B|^{3/4}\sqrt{\pi}}{\sqrt{a}}\ e^{-2\sqrt{|E_B|}a}\ , \tag{137}$$

which should be compared with the usual one-dimensional double well potential splitting given in the introduction. Note that in the former case, the strength of each harmonic well is proportional to the square of the separation therefore the initial energy level is not independent as in the delta function case and is proportional to the square of the separation. the exponent thus gets the square of the distance as the suppression factor, if we assume that $E_B \sim |a|^2$ one can see that the exponents behave exactly the same way. Actually, one can also compare the first order perturbation result for the splitting δE_1 with the numerical result by solving $\det\Phi(\nu) = \ln(\nu/\mu) - \pm K_0(2a\nu) = 0$ numerically for each a by Mathematica (see **Figure 2**). We assume that $a > e^\gamma$ in order to guarantee the existence of the second bound states, where γ is the Euler's constant.

The same method can also be applied to the one-dimensional case. In the symmetrically placed Dirac delta potentials with equal strengths λ, the exact bound state energies when they are sufficiently far away from each other (when $a > 1/\lambda$, there are two bound state energies) can analytically be computed [41]

$$E_\pm = -\left(\frac{\lambda}{2} + \frac{1}{2a}W\left(\pm a\lambda e^{-a\lambda}\right)\right)^2\ , \tag{138}$$

where W is the Lambert W function [42], which is defined as the solution $y(x)$ of the transcendental equation $ye^y = x$. From (17), the principal matrix in this case reads

$$\Phi_{ij}(E) = \begin{cases}\frac{1}{\lambda} - \frac{1}{2\sqrt{-E}} & \text{if } i = j\\ -\frac{1}{2\sqrt{-E}}e^{-2a\sqrt{-E}} & \text{if } i \neq j\end{cases}\ . \tag{139}$$

Then, the first order perturbation result following the above procedure gives

$$\delta E_1 = \lambda^2 e^{-a\lambda}\ , \tag{140}$$

where we have used well-known result $E_B = -\frac{\lambda^2}{4}$. Then, one can easily find the error between the exact result $\delta E_{exact} = E_+ - E_-$ and the first order perturbation result δE_1 in the splitting of the energy, see the **Figure 3**.

The three dimensional case can also be studied in this way and we can similarly solve $\det\Phi(\nu) = (\nu - \mu) - \pm\frac{1}{2a}e^{-2a\nu}$ in terms

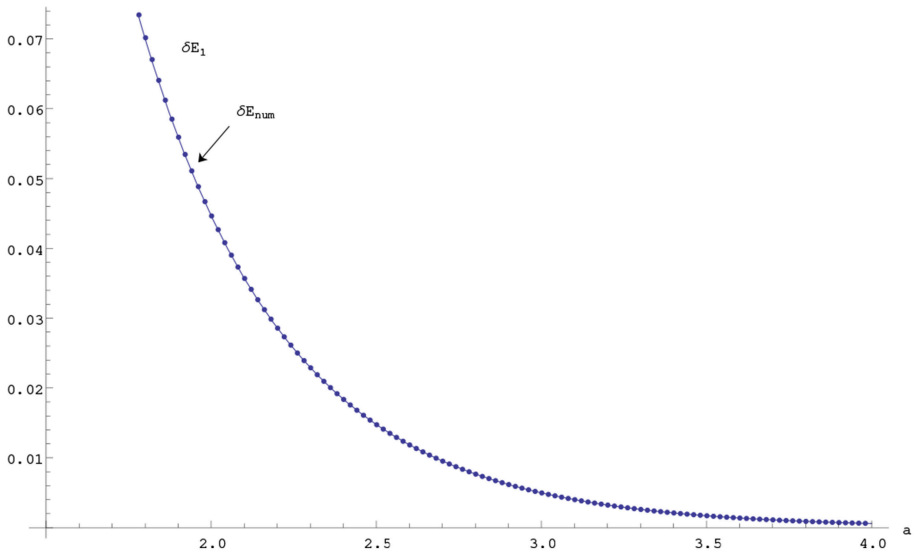

FIGURE 2 | Numerical and first order perturbation results for the splitting in the energy as a function of a for $\mu = 1$ unit in two dimensions.

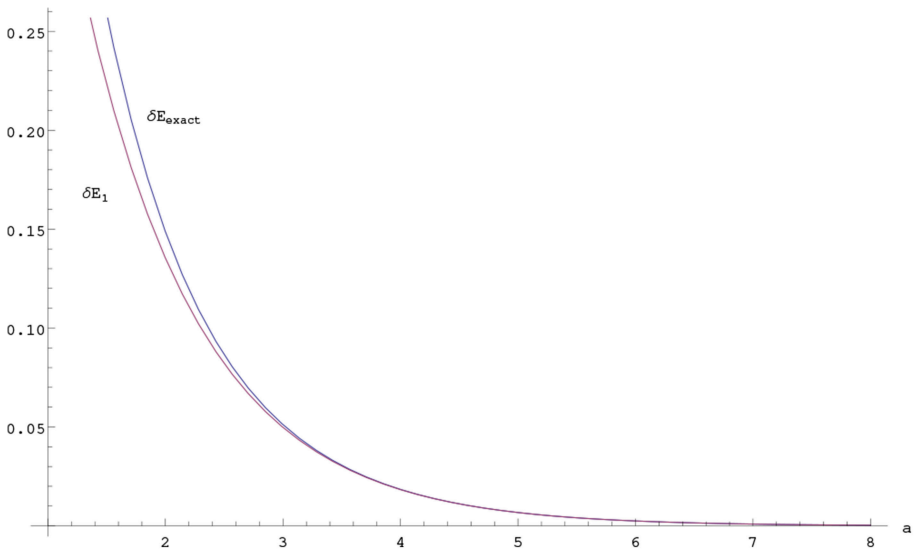

FIGURE 3 | Exact and first order perturbation results for the splitting in the energy as a function of a for $\lambda = 1$ unit in one dimension.

of the Lambert W function and compare with the first order perturbation result for the splitting in the energy (**Figure 4**):

Here we assume that $a > 1/2\mu$ in order to guarantee the existence of second bound states.

Let us emphasize that in the usual WKB approach one constructs the wave functions in classically allowed and forbidden regions respectively and use a subtle argument to connect the different regions. In this case, there is really no forbidden region, except the supports of the attractive regions. Indeed right here classically there is no sensible way to define the motion of a particle. Nevertheless, it is possible to find the effect of tunneling for the wave functions from our formalism. It relies on the first order corrections to the eigenstates of the principal operator, notice that an expansion of the eigenstates of the principal operator can be found in the non-degenerate case as

$$A^k(E_B^k) = A_0^k(E_B^k) + \sum_{r\neq k} \frac{\langle A_0^k(E_B^k), \delta\Phi_{kr}(E_B^k) A_0^r(E_B^k)\rangle}{\omega_0^k(E_B^k) - \omega_0^r(E_B^k)} A_0^r(E_B^k)\ . \tag{141}$$

Note that to this order the normalization is not important, moreover we do not need to use a subtle argument about the shift of the eigenvalues since the change of eigenvalue is already second order in the exponentially small quantities, any such

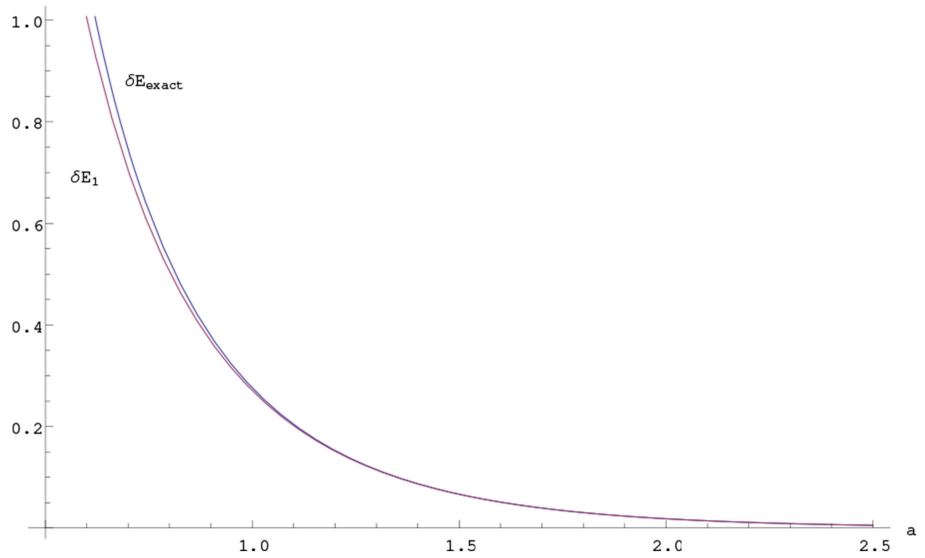

FIGURE 4 | Exact and first order perturbation results for the splitting in the energy as a function of a for $\mu = 1$ unit in three dimensions.

correction will be of lower order as we have seen in the shift of energy calculations.

It is well-known that the wave function of the system associated with the bound states can be found from the explicit expression of the resolvent formula. Since the eigenvalues are isolated we can find the projections onto the subspace corresponding to this eigenvalue by the following contour integral (Riesz Integral representation) [5]:

$$\mathbb{P}_k = -\frac{1}{2\pi i}\oint_{C_k} \mathrm{d}z\, R(z), \tag{142}$$

where C_k is a small contour enclosing the isolated eigenvalue, say E_k. We note that the free resolvent does not contain any poles on the negative real axis for the Dirac delta potentials supported by points, so all the poles on the negative real axis will come from the poles of inverse principal matrix $\Phi^{-1}(z)$. Since the principal matrix is self-adjoint on the real axis, we can apply the spectral theorem. Moreover, its eigenvalues and eigenprojections are holomorphic near the real axis, as emphasized in section 3. Then, we can write the spectral resolution of the inverse principal matrix,

$$\Phi^{-1}_{ij}(z) = \sum_k \frac{1}{\omega^k(z)}\mathbb{P}_k(z)_{ij}\,, \tag{143}$$

where $\mathbb{P}_k(z)_{ij} = \overline{A^{ik}(z)}A^{jk}(z)$, $A^{ki}(z)$ is the normalized eigenvector corresponding to the eigenvalue $\omega^k(z)$. Then, from the residue theorem, we find the square integrable wave function associated with the bound state energy E_k as

$$\psi_k(\mathbf{x}) = \alpha \sum_{i=1}^{N} R_0(\mathbf{x}, \mathbf{a_i}; E_k)\, A^{ki}(E_k)\,, \tag{144}$$

where $\alpha = (-\frac{\partial\omega^k}{\partial E}\big|_{E_k})^{-1/2}$ is the normalization constant. This is actually a general formula for the bound state wave function for the Dirac delta potentials supported by points in $\mathbb{R}^n$. For $n = 2$, we have

$$\psi_k(\mathbf{x}) = \frac{\alpha}{2\pi} \sum_{i=1}^{N} K_0(\sqrt{-E_k}|\mathbf{x} - \mathbf{a_i}|)\, A^{ki}(E_k)\,. \tag{145}$$

Let us recall that the eigenstates for the unperturbed levels are given by unit vectors (103), when we write this into the formula for the wave function (145). As a result, using the first order correction (100) to the eigenstate A^k we find that the change of the wave original wave function in the first order becomes,

$$\begin{aligned}\delta\psi_k(x) &= \frac{(4\pi E_B^k)^{1/2}}{2\pi}\sum_{l\neq k}\frac{1}{\ln(|E_k^B|/|E_l^B|)}K_0(\sqrt{|E_B|}|\mathbf{a_k} - \mathbf{a_l}|)K_0(\sqrt{|E_k^B|}|\mathbf{x} - \mathbf{a_l}|)\\ &\sim \sqrt{2}|E_B^k|^{1/4}\sum_{l\neq k}\frac{1}{\ln(|E_k^B|/|E_B^l|)}\frac{e^{-\sqrt{|E_B^k|}|\mathbf{a_k}-\mathbf{a_l}|}}{\sqrt{|\mathbf{a_k} - \mathbf{a_l}|}}K_0(\sqrt{|E_B^k|}|\mathbf{x} - \mathbf{a_l}|)\,,\end{aligned} \tag{146}$$

where we use

$$\frac{1}{\left(-\frac{\partial\omega_0^k(E)}{\partial E}\Big|_{E_B^k}\right)} = 4\pi|E_B^k|\,. \tag{147}$$

This form of the wave function clearly shows the tunneling nature of the wave functions. It is now quite straightforward to compute the wave functions in this approximation for all the other cases we consider.

CONCLUSION

In this paper, we have first reviewed the basic results about some singular interactions, such as the Dirac delta potentials

supported by points on flat spaces and hyperbolic manifolds, and delta potentials supported by curves in flat spaces. Moreover, the results in the relativistic extensions of the above-mentioned potentials have been also reviewed which was essentially given in Altunkaynak et al. [13], Erman and Turgut [14], Erman [15], Dogan and Turgut [17], Erman et al. [18], and Kaynak and Turgut[19]. The main result of this paper is to develop some kind of perturbation theory applied to some class of singular potentials in order to find the splitting in the energy due to the tunneling. This was only developed for Dirac delta potentials supported by points in Erman and Turgut [14], here we extend the method for various kind of Dirac delta potentials as well as its relativistic extensions.

It is possible to give some bounds over the error terms if we assume that the errors in perturbation theory can be estimated. Typical perturbative expansions are asymptotic therefore a truncation is needed to get more accurate results, one knows that it gets worse beyond a few terms. The more accurate thing to do is to obtain a Borel summed version but that is beyond the content of the present paper, it will depend very much of the specifics of the model whereas we prefer to give a broader perspective.

The comparison with conventional methods certainly would be very useful, nevertheless at present we do not know how a more conventional approach, such as WKB or instanton calculus can be performed in these singular problems. Since the potentials are localized at points or along the curves, the variation of the potential relative to any wavelength is always much more important. Indeed this unusual behavior changes the problem completely. We need to give a meaning to these potentials first and redevelop the WKB analysis. Our main point here is that in this description of the singular potentials via resolvents, the WKB's reincarnation is given by a perturbative analysis of the eigenvalues of the principal operator for large separations of the supports.

DATA AVAILABILITY

All datasets generated for this study are included in the manuscript and/or the supplementary files.

AUTHOR CONTRIBUTIONS

All authors listed have made a substantial, direct and intellectual contribution to the work, and approved it for publication.

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Point Interactions With Bias Potentials

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We develop an approach on how to define single-point interactions under the application of external fields. The essential feature relies on an asymptotic method based on the one-point approximation of multi-layered heterostructures that are subject to bias potentials. In this approach, the zero-thickness limit of the transmission matrices of specific structures is analyzed and shown to result in matrices connecting the two-sided boundary conditions of the wave function at the origin. The reflection and transmission amplitudes are computed in terms of these matrix elements as well as biased data. Several one-point interaction models of two- and three-terminal devices are elaborated. The typical transistor in the semiconductor physics is modeled in the "squeezed limit" as a δ- and a δ'-potential and referred to as a "point" transistor. The basic property of these one-point interaction models is the existence of several extremely sharp peaks as an applied voltage tunes, at which the transmission amplitude is non-zero, while beyond these resonance values, the heterostructure behaves as a fully reflecting wall. The location of these peaks referred to as a "resonance set" is shown to depend on both system parameters and applied voltages. An interesting effect of resonant transmission through a δ-like barrier under the presence of an adjacent well is observed. This transmission occurs at a countable set of the well depth values.

Keywords: one-dimensional quantum systems, transmission, point interactions, resonant tunneling, controllable potentials, heterostructures

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1. INTRODUCTION

One-dimensional quantum systems modeled by Schrödinger operators with singular zero-range potentials have been discussed widely in both the physical and mathematical literature [see books [1–3] for details and references]. Additionally, a whole body of literature beginning from the early publications [4–11] (to mention just a few) has been published, where the one-dimensional stationary Schrödinger equation

$$-\psi''(x) + V(x)\psi(x) = E\psi(x), \tag{1}$$

with the potential $V(x)$ given in the form of distributions, where $\psi(x)$ is the wave function and E the energy of an electron, was shown to exhibit a number of peculiar features with possible applications to quantum physics. Currently, because of the rapid progress in fabricating nanoscale quantum devices, of particular importance is the point modeling of different structures like quantum waveguides [12, 13], spectral filters [14, 15], or infinitesimally thin sheets [16, 17].

In the present paper we follow the traditional approach [see the work [7] by Albeverio et al. and references therein], according to which there exists a one-to-one correspondence between the full set of self-adjoint extensions of the one-dimensional free Schrödinger operator and the two families of boundary conditions: *non-separated* and *separated*. The non-separated extensions describe non-trivial four-parameter point interactions subject to the two-sided at $x = \pm 0$ boundary conditions on the wave function $\psi(x)$ and its derivative $\psi'(x)$ given by the connection matrix of the form

$$\begin{pmatrix} \psi(+0) \\ \psi'(+0) \end{pmatrix} = \Lambda \begin{pmatrix} \psi(-0) \\ \psi'(-0) \end{pmatrix}, \quad \Lambda = \mathrm{e}^{\mathrm{i}\chi} \begin{pmatrix} \lambda_{11} & \lambda_{12} \\ \lambda_{21} & \lambda_{22} \end{pmatrix}, \quad (2)$$

where $\chi \in [0, \pi)$, $\lambda_{ij} \in \mathbb{R}$ fulfilling the condition $\lambda_{11}\lambda_{22} - \lambda_{12}\lambda_{21} = 1$. The separated point interactions are described by the direct sum of the free Schrödinger operators defined on the half-lines $(-\infty, 0)$, $(0, \infty)$ and subject to the following pair of boundary conditions:

$$\psi'(-0) = h^- \psi(-0) \quad \text{and} \quad \psi'(+0) = h^+ \psi(+0), \quad (3)$$

where $h^\pm \in \mathbb{R} \cup \{\infty\}$. For instance, if $\{h^-, h^+\} = \{\infty, \infty\}$, Equation (3) describe the Dirichlet boundary conditions $\psi(\pm 0) = 0$. In physical terms, a separated self-adjoint extension means that the corresponding point potential is completely opaque for an incident particle. Alternatively, the boundary conditions can be connected using the Asorey-Ibort-Marmo formalism [18] or the Cheon-Fülöp-Tsutsui approach [19, 20]. The advantage of both these connecting representations is that they enable to include all the self-adjoint extensions without treating the particular cases as any parameters tend to infinity. In other words, the relations (3) are excluded from the consideration.

Some particular examples of Equation (1) and the corresponding Λ-matrix (2) are important in applications. The most simple and widespread potential is Dirac's delta function $\delta(x)$, i.e., $V(x) = \alpha\delta(x)$ where α is a strength constant (or intensity). The wave function $\psi(x)$ for this interaction (called the δ-interaction or δ-potential) is continuous at the origin $x = 0$, whereas its derivative undergoes a jump, so that the boundary conditions read $\psi(-0) = \psi(+0) =: \psi(0)$ and $\psi'(+0) - \psi'(-0) = \alpha\psi(0)$ yielding the Λ-matrix in the form

$$\Lambda = \begin{pmatrix} 1 & 0 \\ \alpha & 1 \end{pmatrix}. \quad (4)$$

In the simplest case, this point potential is constructed from constant functions defined on a squeezed interval.

The dual point interaction for which the derivative $\psi'(x)$ is continuous at the origin, but $\psi(x)$ discontinuous, is called a δ'-interaction (the notation adopted in the literature [2]). This point interaction with strength β defined by the boundary conditions $\psi'(-0) = \psi'(+0) =: \psi'(0)$ and $\psi(+0) = \psi(-0) = \beta\psi'(0)$ has the Λ-matrix of the form

$$\Lambda = \begin{pmatrix} 1 & \beta \\ 0 & 1 \end{pmatrix}. \quad (5)$$

As a particular example of the Cheon-Shigehara approach [21], the δ'-interaction can be constructed from the spatially symmetric configuration consisting of three separated δ-potentials having the intensities scaled in a non-linear way as the distances between the potentials tend to zero. Following this approach, Exner et al. [22] have approximated the δ-potentials by regular functions and realized rigorously the similar one-point limit in the norm resolvent topology. In particular, they have proved that the resulting limit takes place if the distances between the peaks of δ-like regularized potentials tend to zero sufficiently slow relative to shrinking these potentials to the origin. The other aspects of the δ'-interaction and its approximations by local and non-local potentials have been investigated, for instance, by Albeverio and Nizhnik [23–27], Fassari and Rinaldi [28] (see also references therein). The δ'-interaction can be used together with background potentials. Thus, Albeverio et al. [29] have rigorously defined the self-adjoint Hamiltonian of the harmonic oscillator perturbed by an attractive δ'-interaction of strength β centered at the origin $x = 0$ (the bottom of a confining parabolic potential), explicitly providing its resolvent. In a subsequent publication [30], their study has been extended for the perturbation by a triple of attractive δ'-interactions using the Cheon-Shigehara approximation. It is worth mentioning the recent publication [31], where Golovaty has constructed a new approximation to the δ'-interaction involving two parameters in the boundary conditions. Here the connection matrix

$$\Lambda = \begin{pmatrix} \theta & \beta \\ 0 & \theta^{-1} \end{pmatrix} \quad (6)$$

describes the two-parametric family of point interactions being the generalization of the δ'-interaction with $\theta = 1$.

It should be emphasized that the term "δ'-interaction" is somewhat misleading because the point interaction described by the Λ-matrix (5) does not correspond to Equation (1) in which the potential part is the derivative of the Dirac delta function in the distributional sense, i.e., $V(x) = \gamma\delta'(x)$ with strength γ. Since the term $\delta'(x)\psi(x)$ is not defined for discontinuous $\psi(x)$, Kurasov [5] has developed the distribution theory based on the space of discontinuous at $x = 0$ test functions. Within this theory, as a particular example, the point interaction that corresponds to the potential $V(x) = \gamma\delta'(x)$ is given by the connection matrix

$$\Lambda = \begin{pmatrix} \theta & 0 \\ 0 & \theta^{-1} \end{pmatrix}, \quad (7)$$

where $\theta = (2 + \gamma)/(2 - \gamma)$, $\gamma \in \mathbb{R} \setminus \{\pm 2\}$. Since the term "$\delta'$-interaction" is reserved for the case with the connection matrix of the type (5), Brasche and Nizhnik [32] suggested to refer the point interactions described by the matrices of the form (7) even if the element $\theta \neq 1$ does not correspond to the delta prime potential. We will follow this terminology in the present paper.

The Kurasov approach has been followed in many applications (see, e.g., [32–39]) including more general examples. Thus, in the context of this approach, Gadella et al. [33] have shown that Equation (1) with the potential $V(x) = a\delta(x) + b\delta'(x)$, $a < 0$, $b \in \mathbb{R}$, has a bound state and calculated the energy of

this state in terms of the parameters a and b. A new approach based on the integral form of the Schrödinger Equation (1) has been developed by Lange [35, 36] with some revision of Kurasov's theory. The potential $V(x) = a\delta(x) + b\delta'(x)$ has also been used by Gadella and coworkers as a perturbation of some background potential, such as a constant electric field and the harmonic oscillator [34] or the infinite square well [37]. The spectrum of a one-dimensional V-shaped quantum well perturbed by three types of a point impurity as well as three solvable two-dimensional systems (the isotropic harmonic oscillator, a square pyramidal potential and their combination) perturbed by a point interaction centered at the origin has been studied by Fassari et al. in the recent papers [40–42].

On the other hand, as derived in the series of publications [43–47] for some particular cases and proved rigorously by Golovaty with coworkers [48–52] in a general case, the potential $V(x) = \gamma\delta'(x)$ appears to be partially transparent at some discrete values forming a countable set $\{\gamma_n\}$ in the γ-space. The corresponding Λ-matrix is diagonal, i.e., of the form (7) where the element $\theta = \{\theta_n\}$ takes discrete values that depend on the sequence $\{\gamma_n\}$. Except the distribution $\delta'(x)$, which is obtained as a limit of regular δ'-like functions, the diagonal form of the Λ-matrix can be realized even if the squeezed limit of regular functions does not exist. Beyond the "resonance" set $\{\gamma_n\}$, the δ'-potential is fully opaque satisfying the boundary conditions of the type (3). However, this resonant-tunneling behavior contradicts with the Λ-matrix (7) where the element θ continuously depends on strength γ. It is remarkable that this controversy can be resolved using the one-dimensional model for the heterostructure consisting of two or three squeezed parallel homogeneous layers approaching to one point [53, 54]. Here a "splitting" effect of one-point interactions has been described.

As for two-point interactions in one dimension, one should mention the recent studies concerning quantum tunneling times and the associated questions such as, for instance, the Hartman effect and its generalized version [see, e.g., [55–59] and references therein]. Another important aspect regarding the application of double-point potentials is the Casimir effect that arises in the behavior of the vacuum energy between two homogeneous parallel plates. For the interpretation of this effect, Muñoz-Castañeda and coworkers [60–66] reformulated the theory of self-adjoint extensions of symmetric operators over bounded domains in the framework of quantum field theory. Particularly, they have calculated the vacuum energy and identified which boundary conditions generate attractive or repulsive Casimir forces between the plates. Bordag and Muñoz-Castañeda [67] have calculated the quantum vacuum interaction energy between two kinks of the sine-Gordon equation (for a review on nonlinear localized excitations including topological solitons see, e.g., the work [68]) and shown that this interaction induces an attractive force between the kinks in parallel to the Casimir force between conducting mirrors. A rigorous mathematical model of real metamaterials has been suggested in Nieto et al. [69]. The resonant tunneling through double-barrier scatters is still an active area of research for the applications to nanotechnology. In the context of the Cheon-Fülöp-Tsutsui approach [19, 20], the conditions for the parameter space under which the perfect resonant transmission occurs through two point interactions, each of which is described by four parameters, have been found by Konno et al. [70, 71].

The pioneering studies [72–74] demonstrated that the resonant transmission through quantum multilayer heterostructures of electronic tunnel systems are of considerable general interest. These structures are not only important in micro- and nanodevices, but their study involves a great deal of basic physics. In recent years it has been realized that the study of the electron transmission through heterostructures can be investigated in the zero-thickness limit approximation materialized when their width shrinks to zero. Within such an approximation it is possible to produce various point interaction models, particularly those as described above which admit exact closed analytic solutions. These models are required to provide relatively simple configurations where an appropriate way of squeezing to the zero-width limit must be compatible with the original real structure. Additionally, as a rule, the nanodevices are subject to electric fields applied externally. In this regard, is of great interest to produce point interaction models with bias potentials. So far no models have been elaborated for such devices using one-point approximation methods.

The present paper is devoted to the investigation of planar heterostructures composed of extremely thin layers separated by small distances in the limit where both the layer thickness and the distance between the layers simultaneously tend to zero. The electron motion in the systems of this type is usually confined in the longitudinal direction (say, along the x-axis); the latter is perpendicular to the transverse planes where electronic motion is free. The three-dimensional Schrödinger equation of such a structure can be separated into longitudinal and transverse parts, writing the total electron energy as the sum of the longitudinal and transverse energies: $E_l + \hbar^2\mathbf{k}_t^2/2m^*$, where m^* is an effective electron mass and $\mathbf{k}_t$ the transverse wave vector; for such additive Hamiltonian the wave function is expressed as a product, i.e. $\psi = \psi_l\psi_t$. As a result, we arrive at the reduced one-dimensional Schrödinger equation with respect to the longitudinal component of the wave function $\psi_l(x)$ and the electron energy E_l. For brevity of notations, in the following we omit the subscript "l" at both $\psi_l(x)$ and E_l. Thus, in the units as $\hbar^2/2m^* = 1$, the one-dimensional stationary Schrödinger equation reduces to the form (1) where $V(x)$ is a potential for electrons. Concerning the dimensions of the longitudinal electron position x, the potential $V(x)$ and the electron energy E, in the system $\hbar^2/2m^* = 1$ we have $[x]$ = nm and $[V, E]$ = nm^{-2}. For computations we choose $m^* = 0.1\, m_e$ and in this case, 1 eV = 2.62464 nm^{-2}.

2. TRANSMISSION CHARACTERISTICS OF MULTI-LAYERED STRUCTURES

This introductory section generalizes the approach described in Lui and Fukuma [75]. We consider the Schrödinger Equation (1), where the potential $V(x)$ is an arbitrary piecewise function defined on the interval (x_0, x_N) with N subsets (x_{i-1}, x_i), $i = \overline{1, N}$, $N = 1, 2, \ldots$. Each $V_i(x)$ is a real bounded function

defined on this interval, so that we have the set of functions: $V_1(x), \ldots, V_N(x)$. Next, we express the transmission matrix in terms of the interface values of the linearly independent solutions of the Schrödinger equation.

The solution of the Schrödinger equation across the interval (x_{i-1}, x_i), $\psi_i(x)$, will be given as

$$\psi_i(x) = C_i^{(1)} u_i(x) + C_i^{(2)} v_i(x), \ \ \overline{1, N}, \tag{8}$$

where $u_i(x)$ and $v_i(x)$ are linearly independent solutions on the interval (x_{i-1}, x_i). At the interface x_i, $i = \overline{1, N-1}$, the particle conservation requires the continuity of the wave function $\psi(x)$, while the momentum conservation demands the continuity of the first derivative of the wave function $\psi'(x)$ resulting in the equations

$$\psi_i(x_i) = \psi_{i+1}(x_i), \ \ \psi_i'(x_i) = \psi_{i+1}'(x_i), \ \ i = \overline{1, N-1}, \tag{9}$$

where the prime denotes first derivative with respect to x.

2.1. Transmission Matrix

Using Equation (8), the boundary conditions (9) can be realized as a system of two linear equations with two unknowns such that

$$\mathbf{M}_i(x_i)\mathbf{C}_i = \mathbf{M}_{i+1}(x_i)\mathbf{C}_{i+1}, \quad i = \overline{1, N-1}, \ \ N \geq 2, \tag{10}$$

where

$$\mathbf{C}_i := \mathrm{col}\left(C_i^{(1)}, C_i^{(2)}\right) = \begin{pmatrix} C_i^{(1)} \\ C_i^{(2)} \end{pmatrix} \ \text{and} \ \mathbf{M}_i(x) := \begin{pmatrix} u_i(x) & v_i(x) \\ u_i'(x) & v_i'(x) \end{pmatrix} \tag{11}$$

are Wronskian matrices. Next, using Equation (10), one can connect the column vectors $\mathbf{C}_1$ and $\mathbf{C}_N$ as follows

$$\begin{aligned} \mathbf{C}_N &= \mathbf{M}_N^{-1}(x_{N-1})\mathbf{M}_{N-1}(x_{N-1})\mathbf{M}_{N-1}^{-1}(x_{N-2}) \ldots \mathbf{M}_2(x_2)\mathbf{M}_2^{-1}(x_1)\mathbf{M}_1(x_1)\mathbf{C}_1 \\ &= \mathbf{M}_N^{-1}(x_{N-1})\Lambda_{N-1}(x_{N-2}, x_{N-1}) \ldots \Lambda_2(x_1, x_2)\mathbf{M}_1(x_1)\mathbf{C}_1, \ \ N \geq 2, \end{aligned} \tag{12}$$

where we have introduced the following matrices:

$$\Lambda_i(x_{i-1}, x_i) := \mathbf{M}_i(x_i)\mathbf{M}_i^{-1}(x_{i-1}), \quad i = \overline{2, N-1}, \ \ N \geq 3. \tag{13}$$

Here each matrix $\Lambda_i(x_{i-1}, x_i)$ connects the boundary values of the corresponding Wronskian matrix $\mathbf{M}_i(x)$ at $x = x_{i-1}$ and $x = x_i$. Yet, it is not obvious that the matrices Λ_i's are transmission matrices connecting the boundary conditions imposed on the wave functions $\psi_i(x)$ at $x = x_{i-1}$ and $x = x_i$. To prove this fact, we compute the right-hand matrix product of (13) and obtain

$$\Lambda_i(x_{i-1}, x_i) = \begin{pmatrix} \lambda_{i,11} & \lambda_{i,12} \\ \lambda_{i,21} & \lambda_{i,22} \end{pmatrix}, \tag{14}$$

where

$$\begin{aligned} \lambda_{i,11}(x_{i-1}, x_i) &= \left[u_i(x_i)v_i'(x_{i-1}) - u_i'(x_{i-1})v_i(x_i)\right]/W_i, \\ \lambda_{i,12}(x_{i-1}, x_i) &= \left[u_i(x_{i-1})v_i(x_i) - u_i(x_i)v_i(x_{i-1})\right]/W_i, \\ \lambda_{i,21}(x_{i-1}, x_i) &= \left[u_i'(x_i)v_i'(x_{i-1}) - u_i'(x_{i-1})v_i'(x_i)\right]/W_i, \\ \lambda_{i,22}(x_{i-1}, x_i) &= \left[u_i(x_{i-1})v_i'(x_i) - u_i'(x_i)v_i(x_{i-1})\right]/W_i, \end{aligned} \tag{15}$$

with the Wronskian

$$W_i = W_i(x_{i-1}) = u_i(x_{i-1})v_i'(x_{i-1}) - u_i'(x_{i-1})v_i(x_{i-1}) \tag{16}$$

computed at $x = x_{i-1}$, which does not depend on x on the interval (x_{i-1}, x_i). Using Equations (15) and (16), one can check the equality

$$|\Lambda_i| = \lambda_{i,11}\lambda_{i,22} - \lambda_{i,12}\lambda_{i,21} = 1. \tag{17}$$

There is an infinite number of the linearly independent solutions $u_i(x)$ and $v_i(x)$. The representation of the Λ_i-matrix elements can be simplified if we choose these solutions satisfying the initial conditions:

$$u_i(x_{i-1}) = 1, \ \ u_i'(x_{i-1}) = 0, \ \ v_i(x_{i-1}) = 0, \ \ v_i'(x_{i-1}) = 1. \tag{18}$$

Inserting thus these conditions into Equations (15) and (16), we get that $W_i = 1$ and, as a result,

$$\Lambda_i(x_{i-1}, x_i) = \begin{pmatrix} u_i(x_i) & v_i(x_i) \\ u_i'(x_i) & v_i'(x_i) \end{pmatrix}. \tag{19}$$

The next step is to compute the product $\Lambda_i(x_{i-1}, x_i)\mathrm{col}\left(\psi_i(x_{i-1}), \psi_i'(x_{i-1})\right)$. This computation immediately results in $\mathrm{col}\left(\psi_i(x_i), \psi_i'(x_i)\right)$, so that we have the matrix relation

$$\begin{pmatrix} \psi_i(x_i) \\ \psi_i'(x_i) \end{pmatrix} = \Lambda_i(x_{i-1}, x_i) \begin{pmatrix} \psi_i(x_{i-1}) \\ \psi_i'(x_{i-1}) \end{pmatrix}, \tag{20}$$

confirming that Equation (13) indeed defines the transmission matrix $\Lambda_i(x_{i-1}, x_i)$ expressed in terms of the matrices $\mathbf{M}_i(x_{i-1})$ and $\mathbf{M}_i(x_i)$. Thus, each transmission matrix $\Lambda_i(x_{i-1}, x_i)$ connects the boundary conditions at $x = x_{i-1}$ and $x = x_i$.

Equation (12) that connects the column vectors $\mathbf{C}_1$ and $\mathbf{C}_N$ can be transformed to the equation connecting the boundary conditions at $x = x_0$ and $x = x_N$. To this end, we define the lateral transmission matrices $\Lambda_i(x_{i-1}, x_i)$ with $i = 0, N$. Thus, on one side, one can write

$$\mathbf{M}_1(x_1)\mathbf{C}_1 = \begin{pmatrix} \psi_1(x_1) \\ \psi_1'(x_1) \end{pmatrix} = \Lambda_1(x_0, x_1) \begin{pmatrix} \psi_1(x_0) \\ \psi_1'(x_0) \end{pmatrix}. \tag{21}$$

On the other hand, multiplying from the left Equation (12) by $\mathbf{M}_N(x_N)$ and using that

$$\mathbf{M}_N(x_N)\mathbf{C}_N = \begin{pmatrix} \psi_N(x_N) \\ \psi_N'(x_N) \end{pmatrix}, \tag{22}$$

one finds the relation that connects the boundary conditions at $x = x_0$ and $x = x_N$:

$$\begin{pmatrix} \psi_N(x_N) \\ \psi_N'(x_N) \end{pmatrix} = \Lambda(x_0, x_N) \begin{pmatrix} \psi_1(x_0) \\ \psi_1'(x_0) \end{pmatrix} \tag{23}$$

with

$$\Lambda(x_0, x_N) = \Lambda_N(x_{N-1}, x_N) \dots \Lambda_1(x_0, x_1). \quad (24)$$

Thus, the transmission matrix for each layer defined on the interval (x_{i-1}, x_i) can be computed through the solutions $u_i(x)$ and $v_i(x)$ and their derivatives taken at the boundaries $x = x_{i-1}$ and $x = x_i$, resulting in the elements given by Equations (15) and (16).

2.2. Reflection-Transmission Coefficients

Consider now the solutions outside the interval (x_0, x_N). In the region $x < x_0$ and $x > x_N$ where the potential is a constant, the wave function is the well-known free particle solution of the Schrödinger Equation (1) as follows

$$\psi_0(x) = A_1 \exp[ik_L(x - x_0)] + A_2 \exp[-ik_L(x - x_0)] \quad (25)$$

for $x < x_0$ and

$$\psi_{N+1}(x) = B_1 \exp[ik_R(x - x_N)] + B_2 \exp[-ik_R(x - x_N)] \quad (26)$$

for $x > x_N$, where $k_L := \sqrt{E - V_L}$ and $k_R := \sqrt{E - V_R}$. Then the continuity of the boundary conditions at $x = x_0$ and $x = x_N$ leads to the following equations:

$$\begin{aligned} &\psi_0(x_0) = \psi_1(x_0), \;\; \psi_0'(x_0) = \psi_1'(x_0), \\ &\psi_N(x_N) = \psi_{N+1}(x_N), \;\; \psi_N'(x_N) = \psi_{N+1}'(x_N), \end{aligned} \quad (27)$$

which can be represented in the matrix form as follows

$$\mathbf{M}_L\mathbf{A} = \mathbf{M}_1(x_0)\mathbf{C}_1, \quad \mathbf{M}_N(x_N)\mathbf{C}_N = \mathbf{M}_R\mathbf{B}, \quad (28)$$

where $\mathbf{A} := \mathrm{col}(A_1, A_2)$, $\mathbf{B} := \mathrm{col}(B_1, B_2)$ and

$$\mathbf{M}_L := \begin{pmatrix} 1 & 1 \\ ik_L & -ik_L \end{pmatrix}, \quad \mathbf{M}_R := \begin{pmatrix} 1 & 1 \\ ik_R & -ik_R \end{pmatrix}. \quad (29)$$

Using these matrix equations in Equation (12), we obtain the following basic equation, which allows us to represent the reflection-transmission coefficients through the elements (15) of the transmission matrix $\Lambda(x_0, x_N)$:

$$\Lambda(x_0, x_N)\mathbf{M}_L\mathbf{A} = \mathbf{M}_R\mathbf{B}. \quad (30)$$

Thus, if there is no incidental particle coming from the right, one can set

$$A_1 = 1, \;\; A_2 = R_L, \;\; B_1 = T_L, \;\; B_2 = 0, \quad (31)$$

so that in Equation (30) we have $\mathbf{A} = \mathrm{col}(1, R_L)$ and $\mathbf{B} = \mathrm{col}(T_L, 0)$. Similarly, if there is no incidental particle from the left, we put

$$A_1 = 0, \;\; A_2 = T_R, \;\; B_1 = R_R, \;\; B_2 = 1, \quad (32)$$

hence $\mathbf{A} = \mathrm{col}(0, T_R)$ and $\mathbf{B} = \mathrm{col}(R_R, 1)$ in (30). Then Equation (29) becomes a set of two linear equations with respect to the pair $\{R_L, T_L\}$ or $\{R_R, T_R\}$. Solving these equations and using the relation $\lambda_{11}\lambda_{22} - \lambda_{12}\lambda_{21} = 1$, we find

$$R_L = -\frac{p + iq}{D}, \;\; T_L = \frac{2k_L/k_R}{D}, \;\; R_R = \frac{p - iq}{D}, \;\; T_R = \frac{2}{D}, \quad (33)$$

where

$$p := \lambda_{11} - (k_L/k_R)\lambda_{22}\,, \quad q := k_L\lambda_{12} + k_R^{-1}\lambda_{21} \quad (34)$$

and

$$D := \lambda_{11} + (k_L/k_R)\lambda_{22} - i(k_L\lambda_{12} - k_R^{-1}\lambda_{21}). \quad (35)$$

The current $j(x) = (i/2)(\psi\,\partial_x\psi^* - \psi^*\partial_x\psi)$ has to be conserved across the transition region $x_0 \le x \le x_N$. Using the definition of the reflection-transmission coefficients given above, we find the left-to-right current $j_L(x_0) = k_L(1 - |R_L|^2)$, $j_L(x_N) = k_R|T_L|^2$ and the right-to-left current $j_R(x_0) = -k_L|T_R|^2$, $j_R(x_N) = -k_R(1 - |R_R|^2)$. From the equations $j_{L,R}(x_0) = j_{L,R}(x_N)$ we obtain the conservation law for both the directions of the current: $\mathcal{R}_{L,R} + \mathcal{T}_{L,R} = 1$, where

$$\mathcal{R}_L := |R_L|^2, \;\; \mathcal{T}_L := (k_R/k_L)|T_L|^2, \;\; \mathcal{R}_R := |R_R|^2, \;\; \mathcal{T}_R := (k_L/k_R)|T_R|^2. \quad (36)$$

One can derive that $|D|^2 = 4k_L/k_R + p^2 + q^2$ and, as a result, the reflection-transmission amplitudes can be represented in the form

$$\mathcal{R}_{L,R} = \frac{p^2 + q^2}{4k_L/k_R + p^2 + q^2}\,, \quad \mathcal{T}_{L,R} = \frac{4k_L/k_R}{4k_L/k_R + p^2 + q^2}\,. \quad (37)$$

In its turn, the scattering matrix can also be represented in terms of the elements of the transmission matrix Λ. Indeed, due to Equations (33) and (36), this representation reads

$$S = \begin{pmatrix} R_L & \sqrt{k_L/k_R}\,T_R \\ \sqrt{k_R/k_L}\,T_L & R_R \end{pmatrix} = \frac{1}{D}\begin{pmatrix} -p - iq & 2\sqrt{k_L/k_R} \\ 2\sqrt{k_L/k_R} & p - iq \end{pmatrix}, \quad (38)$$

where p, q and D are defined by Equations (34) and (35).

3. SCHRÖDINGER EQUATION AND TRANSMISSION MATRIX FOR THE LAYER WITH A LINEAR POTENTIAL PROFILE

Consider now the particular case of a linear potential profile for the layer defined on the interval (x_{i-1}, x_i). In this case the solutions $u_i(x)$ and $v_i(x)$ and thus the transmission matrix $\Lambda_i(x_{i-1}, x_i)$ can be written explicitly. The Schrödinger Equation (1) for the ith layer, $i = \overline{1, N}$, can be rewritten as

$$-\psi_i''(x) + V_i(x)\psi_i(x) = E\psi_i(x), \quad (39)$$

where the potential $V_i(x)$ is a linear function defined on the interval $x_{i-1} < x < x_i$ of length $l_i := x_i - x_{i-i}$, i.e.,

$$V_i(x) = \eta_i(x - x_i) + V_i(x_i), \;\; \eta_i := \frac{V_i(x_i) - V_i(x_{i-1})}{l_i}\,. \quad (40)$$

These equations can be transformed to the Airy equation

$$\frac{d^2\psi_i(z_i)}{dz_i^2} - z_i\psi_i(z_i) = 0, \tag{41}$$

by setting $z_i(x) = \sigma_i(x - s_i)$, where the constants σ_i and s_i are given by

$$\sigma_i = \eta_i^{1/3}, \quad s_i = x_i + \eta_i^{-1}[E - V_i(x_i)]. \tag{42}$$

According to the general expressions (15), we use the Airy functions of the first and the second order as linearly independent solutions to Equation (41), setting $u_i(x) = Ai(z_i(x))$ and $v_i(x) = Bi(z_i(x))$. On the interval $-\infty < z_i < \infty$, these solutions are real-valued. The interface (boundary) values of the (dimensionless) function $z_i(x)$ at the edges of the ith layer, to be used in Equations (15) and (16), are

$$\begin{aligned} z_{i,i-1} := z_i(x)|_{x=x_{i-1}} &= -\eta_i^{-2/3}k_{i,i-1}^2, \\ z_{i,i} := z_i(x)|_{x=x_i} &= -\eta_i^{-2/3}k_{i,i}^2, \end{aligned} \tag{43}$$

where

$$\begin{aligned} &k_{i,i-1} := \sqrt{E - V_{i,i-1}}\,,\ k_{i,i} := \sqrt{E - V_{i,i}}\,,\ V_{i,i-1} \\ &:= V_i(x_{i-1}),\ V_{i,i} := V_i(x_i). \end{aligned} \tag{44}$$

The Wronskian with respect to the variable z is $W\{Ai(z), Bi(z)\} = 1/\pi$, therefore with respect to x, it is $W\{Ai(z_i(x)), Bi(z_i(x))\} = \sigma_i/\pi$. Then the elements of the Λ_i-matrix are

$$\begin{aligned} \lambda_{i,11}(x_{i-1}, x_i) &= \pi\left[Ai(z_{i,i})Bi'(z_{i,i-1}) - Ai'(z_{i,i-1})Bi(z_{i,i})\right], \\ \lambda_{i,12}(x_{i-1}, x_i) &= (\pi/\sigma_i)\left[Ai(z_{i,i-1})Bi(z_{i,i}) - Ai(z_{i,i})Bi(z_{i,i-1})\right], \\ \lambda_{i,21}(x_{i-1}, x_i) &= \sigma_i\pi\left[Ai'(z_{i,i})Bi'(z_{i,i-1}) - Ai'(z_{i,i-1})Bi'(z_{i,i})\right], \\ \lambda_{i,22}(x_{i-1}, x_i) &= \pi\left[Ai(z_{i,i-1})Bi'(z_{i,i}) - Ai'(z_{i,i})Bi(z_{i,i-1})\right], \end{aligned} \tag{45}$$

where the prime denotes the differentiation with respect to z.

In the $\eta_i \to 0$ limit as $V_i(x_{i-1}) \to V_i(x_i)$, we obtain

$$z_i(x) \to -\sigma_i s_i = \sigma_i\left[-x_i - \frac{E - V_i(x_i)}{\sigma_i^3}\right] \to \sigma_i^{-2}\left[V_i(x_i) - E\right], \tag{46}$$

yielding Equation (39) with a constant profile $V_i(x) \equiv V_i$. In this limit case, one can choose the linearly independent solutions to Equation (39) as

$$\begin{aligned} &u_i(x) = \cos[k_i(x - x_{i-1})], \\ &v_i(x) = k_i^{-1}\sin[k_i(x - x_{i-1})],\ k_i := \sqrt{k^2 - V_i}\,, \end{aligned} \tag{47}$$

satisfying the initial conditions (18). Therefore, due to Equations (19) and (47), the Λ_i-matrix becomes

$$\Lambda_i(x_{i-1}, x_i) = \begin{pmatrix} \cos(k_i l_i) & k_i^{-1}\sin(k_i l_i) \\ -k_i\sin(k_i l_i) & \cos(k_i l_i) \end{pmatrix}. \tag{48}$$

4. ASYMPTOTIC REPRESENTATIONS OF THE SINGLE-LAYER TRANSMISSION MATRIX

Similarly to the previous section, here we also focus on one of the layers and for brevity of notations we replace for while in the above expressions the subscripts $\{i, i-1\}$ and $\{i, i\}$ by "0" and "1", respectively. Then, according to Equations (43) and (44), we write

$$\begin{aligned} z_0 &= -\left(\frac{l}{V_1 - V_0}\right)^{2/3}k_0^2, z_1 = -\left(\frac{l}{V_1 - V_0}\right)^{2/3}k_1^2, \\ \sigma &= \left(\frac{V_1 - V_0}{l}\right)^{1/3}, \end{aligned} \tag{49}$$

where we have replaced $V_{i,i-1}$, $V_{i,i}$, $k_{i,i-1}$, $k_{i,i}$ by V_0, V_1, k_0, k_1, respectively. Using next the two asymptotic expressions for the Airy functions and their derivatives known in the limit as $z \to 0$ and $z \to \pm\infty$, below we will derive the corresponding asymptotic representations of the elements (45) in the two limits as (i) $z_0, z_1 \to 0$ and (ii) $z_0, z_1 \to \pm\infty$. It is reasonable to assume that everywhere z_0 and z_1 are of the same sign. We omit for a while the subscript "i" for the matrix Λ_i and its elements.

4.1. Asymptotic Representation of the Λ-Matrix in the Limit as $z_0, z_1 \to 0$

For the $z_0, z_1 \to 0$ limit to be carried out in Equation (45), one can use the series representation of the Airy functions and their first derivatives in the neighborhood of the origin $z = 0$. It is sufficient to explore only the two first terms:

$$\begin{aligned} Ai(z) &\to \frac{1}{3^{2/3}\Gamma(2/3)} - \frac{z}{3^{1/3}\Gamma(1/3)} + \ldots, \\ Ai'(z) &\to -\frac{1}{3^{1/3}\Gamma(1/3)} + \frac{z^2}{2\cdot 3^{2/3}\Gamma(2/3)} + \ldots, \\ Bi(z) &\to \frac{1}{3^{1/6}\Gamma(2/3)} + \frac{3^{1/6}z}{\Gamma(1/3)} + \ldots, \\ Bi'(z) &\to \frac{3^{1/6}}{\Gamma(1/3)} + \frac{z^2}{2\cdot 3^{1/6}\Gamma(2/3)} + \ldots. \end{aligned} \tag{50}$$

As a result of applying these expansion formulae to Equation (45) and using Euler's reflection formula for the gamma function, $\Gamma(1 - z)\Gamma(z) = \pi/\sin(\pi z)$, $z \notin \mathbb{Z}$, we get the following asymptotic representation of the Λ-matrix elements:

$$\begin{aligned} &\lambda_{11} \to 1 - z_0^2 z_1/2,\ \lambda_{22} \to 1 - z_0 z_1^2/2, \\ &\lambda_{12} \to \frac{z_1 - z_0}{\sigma} = l,\ \lambda_{21} \to \frac{\sigma}{2}(z_1^2 - z_0^2) = -\frac{l}{2}(k_0^2 + k_1^2) \end{aligned} \tag{51}$$

as $z_0, z_1 \to 0$.

4.2. Asymptotic Representation of the Λ-Matrix in the Limit as $z_0, z_1 \to \pm\infty$

In the limit as $z \to -\infty$, for the Airy functions and their derivatives we have the following asymptotics:

$$Ai(z) \to \frac{\sin\left[\frac{2}{3}(-z)^{3/2}+\pi/4\right]}{\sqrt{\pi}(-z)^{1/4}}, \quad Bi(z) \to \frac{\cos\left[\frac{2}{3}(-z)^{3/2}+\pi/4\right]}{\sqrt{\pi}(-z)^{1/4}}, \tag{52}$$

$$\begin{aligned} Ai'(z) &\to \frac{\frac{1}{4}(-z)^{-3/4}\sin\left[\frac{2}{3}(-z)^{3/2}+\pi/4\right]-(-z)^{3/4}\cos\left[\frac{2}{3}(-z)^{3/2}+\pi/4\right]}{\sqrt{\pi}(-z)^{1/2}}, \\ Bi'(z) &\to \frac{\frac{1}{4}(-z)^{-3/4}\cos\left[\frac{2}{3}(-z)^{3/2}+\pi/4\right]+(-z)^{3/4}\sin\left[\frac{2}{3}(-z)^{3/2}+\pi/4\right]}{\sqrt{\pi}(-z)^{1/2}}. \end{aligned} \tag{53}$$

Using this asymptotic representation in Equations (45) as $z_0, z_1 \to -\infty$, we obtain

$$\begin{aligned} \lambda_{11} &\to (-z_0)^{1/4}(-z_1)^{-1/4}\cos\chi_- - (4z_0)^{-1}(-z_0)^{-1/4}(-z_1)^{-1/4}\sin\chi_-, \\ \lambda_{12} &\to -\sigma^{-1}(-z_0)^{-1/4}(-z_1)^{-1/4}\sin\chi_-, \\ \lambda_{21} &\to \sigma\,(-z_0)^{-1/2}(-z_1)^{-1/2} \\ &\quad\times\left\{\left[(-z_0)^{3/4}(-z_1)^{3/4}+4^{-2}(-z_0)^{-3/4}(-z_1)^{-3/4}\right]\sin\chi_- \right. \\ &\quad\left.+\,4^{-1}\left[(-z_0)^{3/4}(-z_1)^{-3/4}-(-z_1)^{3/4}(-z_0)^{-3/4}\right]\cos\chi_-\right\}, \\ \lambda_{22} &\to (-z_1)^{1/4}(-z_0)^{-1/4}\cos\chi_- + (4z_1)^{-1}(-z_0)^{-1/4}(-z_1)^{-1/4}\sin\chi_-, \end{aligned} \tag{54}$$

where

$$\chi_- := \frac{2}{3}\left[(-z_1)^{3/2}-(-z_0)^{3/2}\right]. \tag{55}$$

One can check that $|\Lambda| = \lambda_{11}\lambda_{22} - \lambda_{12}\lambda_{21} = 1$. According to Equations (50), this representation corresponds to a well ($V_j < 0$, $j = 0, 1$). However, these formulae can be "continued" to positive values of z_0 and z_1 that correspond to a barrier with $E < V_j$. To prove this, we use the asymptotic representation of the Airy functions and their derivatives in the limit as $z_0, z_1 \to +\infty$:

$$Ai(z) \to \frac{\mathrm{e}^{-\frac{2}{3}z^{3/2}}}{2\sqrt{\pi}z^{1/4}}, \quad Bi(z) \to \frac{\mathrm{e}^{\frac{2}{3}z^{3/2}}}{\sqrt{\pi}z^{1/4}}, \tag{56}$$

$$Ai'(z) \to -\frac{z^{3/4}+\frac{1}{4}z^{-3/4}}{2\sqrt{\pi}z^{1/2}}\,\mathrm{e}^{-\frac{2}{3}z^{3/2}}, \quad Bi'(z) \to \frac{z^{3/4}-\frac{1}{4}z^{-3/4}}{\sqrt{\pi}z^{1/2}}\,\mathrm{e}^{\frac{2}{3}z^{3/2}} \tag{57}$$

and, as a result, we find

$$\begin{aligned} \lambda_{11} &\to (z_0/z_1)^{1/4}\cosh\chi_+ + (4z_0)^{-1}(z_0z_1)^{-1/4}\sinh\chi_+, \\ \lambda_{12} &\to \sigma^{-1}(z_0z_1)^{-1/4}\sinh\chi_+, \\ \lambda_{21} &\to \sigma\,(z_0z_1)^{-1/2}\left\{\left[(z_0z_1)^{3/4}-4^{-2}(z_0z_1)^{-3/4}\right]\sinh\chi_+ \right. \\ &\quad\left.+\,4^{-1}\left[(z_1/z_0)^{3/4}-(z_0/z_1)^{3/4}\right]\cosh\chi_+\right\}, \\ \lambda_{22} &\to (z_1/z_0)^{1/4}\cosh\chi_+ - (4z_1)^{-1}(z_0z_1)^{-1/4}\sinh\chi_+, \end{aligned} \tag{58}$$

where z_0 and z_1 are positive and

$$\chi_+ := \frac{2}{3}\left(z_1^{3/2}-z_0^{3/2}\right). \tag{59}$$

Similarly, for the elements (58) one can also check that $|\Lambda| = 1$. In fact, Equations (58) with (59) appear to coincide with Equations (54) and (55) if we assume that in the latter equations z_0 and z_1 are positive. To show this, we note that $(-z)^{3/2} = \mathrm{i}^3 z^{3/2} = -\mathrm{i}z^{3/2}$ and, as a result, we get the relation $\chi_- = -\mathrm{i}\chi_+$ for positive z_0 and z_1 in both Equations (55) and (59). Next, the elements (58) are obtained from the representation (54) if we note that $(-z_0)^{1/4}(-z_1)^{1/4} = \mathrm{i}(z_0z_1)^{1/4}$, $(-z_0)^{1/2}(-z_1)^{1/2} = -(z_0z_1)^{1/2}$ and $(-z_0)^{3/4}(-z_1)^{3/4} = -\mathrm{i}(z_0z_1)^{3/4}$. Therefore, in the following it is sufficient to consider only the representation given by Equations (54) and (55), being valid for both negative and positive z_0 and z_1.

Using the explicit values for z_0 and z_1 given by Equations (49), the expression (55) for χ_- can be transformed to

$$\chi_- = \mathrm{sgn}(V_0 - V_1)\,k_{1,0}\,l, \tag{60}$$

where

$$k_{1,0} := \frac{2(k_0^2+k_1^2+k_0k_1)}{3(k_0+k_1)}, \quad k_j := \sqrt{E-V_j}\;\; j = 0, 1. \tag{61}$$

Inserting next the expressions (49) and (60) into Equations (54), one can write the elements of the Λ-matrix in terms of k_0 and k_1 as follows

$$\begin{aligned} \lambda_{11} &\to \left(\frac{k_0}{k_1}\right)^{1/2}\cos(\kappa l) + \frac{k_1^2-k_0^2}{4l}k_0^{-5/2}k_1^{-1/2}\sin(k_{1,0}\,l), \\ \lambda_{12} &\to k_0^{-1/2}k_1^{-1/2}\sin(k_{1,0}\,l), \\ \lambda_{21} &\to \frac{3(k_0^2-k_1^2)^2k_{1,0}}{8lk_0^{5/2}k_1^{5/2}}\cos(k_{1,0}\,l) \\ &\quad -k_0^{1/2}k_1^{1/2}\left[1+\left(\frac{k_0^2-k_1^2}{4l}\right)^2k_0^{-3}k_1^{-3}\right]\sin(k_{1,0}\,l), \\ \lambda_{22} &\to \left(\frac{k_1}{k_0}\right)^{1/2}\cos(\kappa l) + \frac{k_0^2-k_1^2}{4l}k_0^{-1/2}k_1^{-5/2}\sin(k_{1,0}\,l), \end{aligned} \tag{62}$$

where $k_{1,0}$ is defined by Equation (61). One can check that the matrix elements (62) together with the argument (61) satisfy the condition $|\Lambda| = 1$. Note that the only restriction for the existence of the representation (62) are the asymptotics $z_0, z_1 \to \pm\infty$. Both k_0 and k_1 are either real-valued or imaginary. In the particular case $V_1 = V_0$ ($k_1 = k_0$), Equations (61) and (62) reduce to the matrix representation (48).

5. REALIZATION OF POINT INTERACTIONS IN THE ZERO-THICKNESS LIMIT FOR ONE LAYER

Keeping in the following the same notations with respect to the subscripts "0" and "1", let us consider the linear potential (40)

rewritten as

$$V(x) = V_0 + \frac{V_1 - V_0}{l}\, x, \;\; V_0,\, V_1 \in \mathbb{R}, \tag{63}$$

on the interval $0 < x < l$, where V_0 and V_1 are the potential values at the left and right edges of the layer with width l. Consider first the case when this potential is constant, i.e., $V_0 = V_1$. A point interaction can be realized in the limit as the layer thickness $l \to 0$, whereas $V_0 \to \pm\infty$. To this end, one can use the parametrization of the potential $V(x) \equiv V_0$ introducing a dimensionless parameter $\varepsilon > 0$ that controls the shrinking of the layer to zero width as $\varepsilon \to 0$. It is natural to consider the power parametrization setting

$$V_0 = a\,\varepsilon^{-\mu}, \;\; l = \varepsilon d, \;\; a \in \mathbb{R}, \;\; \mu,\, d > 0. \tag{64}$$

In the squeezed limit (as $\varepsilon \to 0$), a one-parameter family of point interactions at $x = 0$ is realized. It is determined by the power $\mu \in (0, \infty)$: the transmission is perfect for $\mu \in (0, 1)$, at $\mu = 1$ the potential takes the form of Dirac's delta function $\alpha\delta(x)$ with the transmission matrix (4), where $\alpha = ad$ is the strength of the δ-interaction, and for $\mu \in (1, \infty)$ the interaction acts as a fully reflecting wall satisfying the Dirichlet boundary condition $\psi(\pm 0) = 0$ for the wave function $\psi(x)$.

In the case when the difference $V_1 - V_0$ is non-zero, as shown in **Figure 1**, one deals with two potential values V_0 and V_1 at the layer edges that must tend to infinity in the zero-thickness limit. Both the potential values V_0 and V_1 are supposed to be of the same sign. In general, the rate of this divergence to infinity can differ and therefore the parametrization of the potential (63) should involve two parameters. We introduce the two powers μ and ν, where the parameters μ and ν describe how rapidly the potential V_0 at the left layer edge and the difference $V_1 - V_0$ tend (escape) to infinity as $\varepsilon \to 0$, respectively. The particular case when this difference is a constant not depending on ε can also be included. Thus, we set

$$\begin{aligned} &V_0 = a\varepsilon^{-\mu}, \\ &V_1 = V_0 + b\,\varepsilon^{-\nu},\; 0 < \mu < \infty,\; 0 \le \nu \le \mu,\; a,\, b \in \mathbb{R},\; l = \varepsilon\, d, \end{aligned} \tag{65}$$

including the following two situations in the squeezed limit: (i) $V_1 - V_0$ is constant ($\nu = 0$) and (ii) the "escaping-to-infinity" rate of $V_1 - V_0$ does not exceed the rate of V_0 ($\nu \le \mu$). In the electronics domain the difference $V_1 - V_0$ or b may play the role of a bias voltage.

Due to Equations (43), we have the asymptotics $z_0, z_1 \sim \varepsilon^{2(1+\nu)/3-\mu}$. Consequently, the line $L_{0,\infty} := \{0 < \mu \le 2,\, \nu = 3\mu/2 - 1\}$ separates the asymptotic representations $z_0, z_1 \to 0$ and $z_0, z_1 \to \pm\infty$ on the (μ, ν)-plane as illustrated by the diagram depicted in **Figure 2**. Here, we have the two triangle sets:

$$\begin{aligned} &S_0 := \{0 < \mu < 2,\, \max\{0,\, 3\mu/2 - 1\} < \nu \le \mu\} \\ &\cup\{0 < \mu < 2/3,\, \nu = 0\}, \\ &S_\infty := \{2/3 < \mu \le 2,\, 0 \le \nu < 3\mu/2 - 1\}, \end{aligned} \tag{66}$$

where the asymptotic representations $z_0, z_1 \to 0$ and $z_0, z_1 \to \pm\infty$ take place, respectively. The corresponding angles are formed by the boundary lines: S_0 by $L_{0,1} := \{0 < \mu < 2/3,\, \nu = 0\}$, $L_{0,2} := \{0 < \mu < 2,\, \nu = \mu\}$ and S_∞ by $L_{\infty,1} := \{2/3 < \mu \le 2,\, \nu = 0\}$, $L_{\infty,2} := \{\mu = 2,\, 0 < \nu < 2\}$.

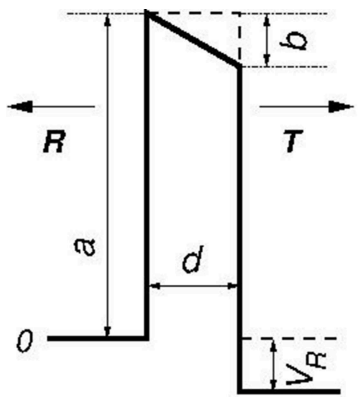

FIGURE 1 | Schematics of one-layer potential (63) tilted by difference $V_1 - V_0$ (solid line) with notations given in (65) at $\varepsilon = 1$: $V_1 - V_0 = b = V_R$. The dashed line represents potential with $b = 0$.

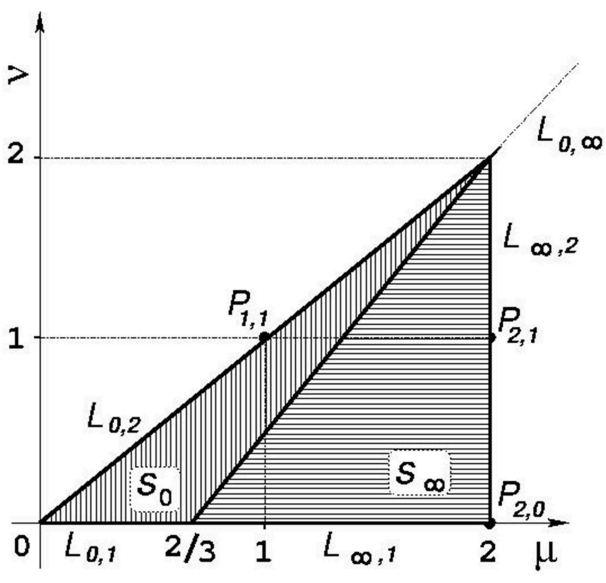

FIGURE 2 | Regions of asymptotic representations $z_0, z_1 \to 0$ (S_0) and $z_0, z_1 \to \pm\infty$ (S_∞) with separating line $L_{0,\infty}$. Three balls indicate characteristic points $P_{1,1} := \{\mu = \nu = 1\} \in S_0$, $P_{2,0} := \{\mu = 2,\, \nu = 0\} \in S_\infty$ and $P_{2,1} := \{\mu = 2,\, \nu = 1\} \in S_\infty$.

5.1. Point Interactions Realized in the Limit as $z_0, z_1 \to 0$

Let us consider the boundary lines $L_{0,1}$ and $L_{0,2}$ of the angle S_0. On the line $L_{0,1}$, we find that $z_0, z_1 \sim \varepsilon^{2/3-\mu}$, so that the $z_0, z_1 \to 0$ limit takes place on the interval $0 < \mu < 2/3$. Next, we have $k_0^2, k_1^2 \sim \varepsilon^{-\mu}$ and according to Equations (51), $\lambda_{12} \to 0$ and $\lambda_{21} \sim \varepsilon^{1-\mu} \to 0$, so that the Λ-matrix becomes the identity ($\Lambda = I$) because $\mu < 1$.

Similarly, on the line $L_{0,2}$, where $z_0, z_1 \sim \varepsilon^{(2-\mu)/3}$, from Equations (49) and (51) we get the asymptotics

$$\begin{aligned} &\lambda_{11} \to 1 - c_1 \varepsilon^{2-\mu}, \ \lambda_{12} \to \varepsilon d, \\ &\lambda_{21} \to (a + b/2) d\, \varepsilon^{1-\mu}, \ \lambda_{22} \to 1 - c_2\, \varepsilon^{2-\mu} \end{aligned} \tag{67}$$

with

$$c_1 := (a^2/2)(a+b)(d/b)^2, \ \ c_2 := (a/2)(a+b)^2(d/b)^2. \tag{68}$$

Therefore, on the interval $0 < \mu < 1$ the transmission matrix is the identity I, while on the interval $1 < \mu < 2$ the transmission matrix does not exist. In this case the point interaction acts as a fully reflecting wall (the boundary conditions for this point interaction are of the Dirichlet type). The value $\mu = 1$ describes the intermediate situation with a partial transmission through the system, namely the δ-interaction with bias b, which separates both these regimes. The limit transmission matrix (as $\varepsilon \to 0$) corresponds to the δ-interaction described by the connection matrix (4) with the strength constant

$$\alpha = (a + b/2)d. \tag{69}$$

This result also includes the constant case when $V_0 = V_1$, i.e., $b = 0$. This approximation is appropriate for modeling the δ-potential. Note that similar analysis can be done for μ and ν belonging to the interior of S_0. In this case in the above equations we have to set $b = 0$.

Using the second formula (37), one can compute the transmission amplitude for this δ-interaction. We get

$$\mathcal{T} = \frac{4k\, k_R}{(k + k_R)^2 + \alpha^2}, \tag{70}$$

where α is given by (69). In the unbiased case ($b = 0$, $k_R = k$) this formula reduces to $\mathcal{T} = \left[1 + (\alpha/2k)^2\right]^{-1}$ with $\alpha = ad$, the well known expression for the constant potential. Equation (70) has been obtained for any $a \in \mathbb{R}$. However, for negative values of a, i.e., for a δ-like well, it does not describe the oscillating behavior with respect to the constant α that takes place under tunneling across a well with finite thickness l.

5.2. Point Interactions Realized in the Limit as $z_0, z_1 \to \pm\infty$

Consider now the characteristic point $P_{2,1} \in S_\infty$ setting in Equation (62) $\mu = 2$ and $\nu = 1$. Here $k_0^2 - k_1^2 = V_1 - V_0 = b\,\varepsilon^{-1}$ and $k_0, k_1, k_{1,0} \to \sqrt{-a}\,\varepsilon^{-1}$, so that the asymptotic representation of Equation (62) in the limit as $\varepsilon \to 0$ becomes

$$\begin{aligned} \lambda_{11} &\to \cos(\kappa d) - \varepsilon\, g \sin(\kappa d), \\ \lambda_{12} &\to \varepsilon\, \kappa^{-1} \sin(\kappa d), \\ \lambda_{21} &\to -\varepsilon^{-1} \kappa \sin(\kappa d) + \mathcal{O}(\varepsilon), \\ \lambda_{22} &\to \cos(\kappa d) + \varepsilon\, g \sin(\kappa d), \end{aligned} \tag{71}$$

where

$$\kappa := \sqrt{-a}, \ \ g := \kappa^{-3}(b/4d). \tag{72}$$

As follows from these asymptotic expressions derived at the point $P_{2,1}$, in the limit as $\varepsilon \to 0$, the transmission through a barrier is zero, while across a well ($a < 0$) it appears to be resonant. The resonance set consists of the roots of the equation $\sin(\kappa d) = 0$. At fixed $d > 0$, these roots form the countable set $\Sigma = \cup_{n=0}^{\infty} \sigma_n$ formed from the points $\sigma_n := -(n\pi/d)^2$. On this resonance set, the discrete-valued matrix is $\Lambda_n := \Lambda|_\Sigma = (-1)^n I$. Beyond these resonance values, the δ-like well is opaque and, instead of the identity matrix I, the two-sided boundary conditions for the wave function are of the Dirichlet type: $(\psi(\pm 0) = 0)$.

6. MULTI-LAYERED HETEROSTRUCTURES WITH BIAS

Now we are ready to apply the expressions obtained above for a single layer to the total structure consisting of an arbitrary number N of layers replacing $\mu \to \mu_i$, $\nu \to \nu_i$, $b \to b_i$, $d \to d_i$. Taking for account that the left boundary value for the potential of the ith layer a_i is shifted because of the biases $b_1, \ldots b_{i-1}$ in the left-hand layers, we need to use the following replacement rule:

$$a \to a_i + \sum_{j=1}^{i-1} b_j, \ \ i = \overline{1, N}, \tag{73}$$

where the sum vanishes if $i = 1$. Then Equation (65) are transformed to

$$\begin{aligned} V_0 \to V_{i,i-1} &= \left(a_i + \sum_{j=1}^{i-1} b_j\right) \varepsilon^{-\mu_i}, \\ V_1 \to V_{i,i} &= V_{i,i-1} + b_i\, \varepsilon^{-\nu_i}. \end{aligned} \tag{74}$$

Next, all the other expressions derived above should be rewritten for the ith layer using the following replacement rules:

$$z_0 \to z_{i,i-1} = \left(\frac{d_i}{b_i}\right)^{2/3} \left[\left(a_i + \sum_{j=1}^{i-1} b_j\right) \varepsilon^{-\mu_i} - E\right] \varepsilon^{2(1+\nu_i)/3},$$

$$z_1 \to z_{i,i} = \left(\frac{d_i}{b_i}\right)^{2/3} \left[\left(a_i + \sum_{j=1}^{i-1} b_j\right) \varepsilon^{-\mu_i} + b_i\, \varepsilon^{-\nu_i} - E\right] \varepsilon^{2(1+\nu_i)/3},$$

$$\alpha \to \alpha_i = \left(a_i + \sum_{j=1}^{i-1} b_j + b_i/2\right) d_i, \ \ \sigma \to \sigma_i = \left(\frac{b_i}{d_i}\right)^{1/3} \varepsilon^{-(1+\nu_i)/3},$$

$$\kappa \to \kappa_i = \sqrt{-\left(a_i + \sum_{j=1}^{i-1} b_j\right)}, \ \ g \to g_i = \frac{b_i}{4\kappa_i^3 d_i},$$

$$c_1 \to c_{i,1} = \frac{1}{2}\left(a_i + \sum_{j=1}^{i-1} b_j\right)^2 \left(a_i + \sum_{j=1}^{i} b_j\right)\left(\frac{d_i}{b_i}\right)^2,$$
$$c_2 \to c_{i,2} = \frac{1}{2}\left(a_i + \sum_{j=1}^{i-1} b_j\right) \left(a_i + \sum_{j=1}^{i} b_j\right)^2 \left(\frac{d_i}{b_i}\right)^2. \quad (75)$$

In the following we will consider some particular examples of multi-layered structures with $N = 2, 3$. It will be shown that in some cases two- and three-lateral quantum devices can be approximated by one-point interactions.

6.1. Two-Layered Structures

Consider now the structure consisting of two layers ($N = 2$). The piecewise linear potential of a barrier-well form is shown in **Figure 3**. For an arbitrary two-layered structure, the limit transmission matrix is the product $\Lambda = \Lambda_2\Lambda_1$, where the matrices Λ_i's can be constructed from the asymptotic approximations (67) and (71) by applying the replacement rules (73)–(75). Applying these rules in Equations (67), (68) and (71), (72) to the matrices Λ_1 and Λ_2, below we compute their product for two different situations. Note that due to the presence of the factor ε^{-1} in the expression λ_{21} [see Equation (71)], the terms of order $\mathcal{O}(\varepsilon)$ must be kept in the product $\Lambda_2\Lambda_1$ because $\lim_{\varepsilon\to 0}\Lambda_2 \cdot \lim_{\varepsilon\to 0}\Lambda_1 \neq \lim_{\varepsilon\to 0}(\Lambda_2\Lambda_1)$.

Point interactions of a δ'-type: Consider the zero-thickness limit determined by the powers $\mu_1 = \mu_2 = 2$ and $\nu_1 = \nu_2 = 1$. Then, the product $\Lambda = \Lambda_2\Lambda_1$ yields the following asymptotic representation of the Λ-matrix elements for the total double-layer system:

$$\begin{aligned}
\lambda_{11} &\to \cos(\kappa_1 d_1)\cos(\kappa_2 d_2) - (\kappa_1/\kappa_2)\sin(\kappa_1 d_1)\sin(\kappa_2 d_2),\\
\lambda_{12} &\to 0,\\
\lambda_{21} &\to \alpha - \varepsilon^{-1}\left[\kappa_1 \sin(\kappa_1 d_1)\cos(\kappa_2 d_2) + \kappa_2 \cos(\kappa_1 d_1)\sin(\kappa_2 d_2)\right],\\
\lambda_{22} &= \cos(\kappa_1 d_1)\cos(\kappa_2 d_2) - (\kappa_2/\kappa_1)\sin(\kappa_1 d_1)\sin(\kappa_2 d_2), \quad (76)
\end{aligned}$$

where the $\varepsilon \to 0$ limit has been performed and

$$\alpha = (\kappa_2 g_1 - \kappa_1 g_2)\sin(\kappa_1 d_1)\sin(\kappa_2 d_2). \quad (77)$$

The second term in the element λ_{21} diverges as $\varepsilon \to 0$ and it vanishes if the equation

$$\kappa_1 \tan(\kappa_1 d_1) + \kappa_2 \tan(\kappa_2 d_2) = 0 \quad (78)$$

takes place. Using this equation in the elements λ_{11} and λ_{22} [see Equation (76)], we find the total transmission matrix

$$\Lambda = \begin{pmatrix} \cos(\kappa_1 d_1)/\cos(\kappa_2 d_2) & 0 \\ \alpha & \cos(\kappa_2 d_2)/\cos(\kappa_1 d_1) \end{pmatrix}. \quad (79)$$

Equation (78) admits a countable set of solutions if at least one of the layer potential has a well profile. In particular, if $a_1 > 0$ (barrier) and $a_2 + b_1 < 0$ (well), Equation (78) reduces to

$$\sqrt{a_1}\tanh(\sqrt{a_1}\, d_1) = \sqrt{|a_2 + b_1|}\tan(\sqrt{|a_2 + b_1|}\, d_2). \quad (80)$$

It is reasonable to assume that $-b_1 < a_1$ (otherwise the right-edge barrier potential becomes negative), so that on the interval $(-a_1, 0)$, under appropriate values of the layer parameters, only a finite set of discrete (resonance) values of b_1 can be found. According to the classification of point interactions given in Brasche and Nizhnik [32], the interactions described by the connection matrix with diagonal elements $\lambda_{11}, \lambda_{22} \neq 1$ may be referred to as a family of (resonant) δ'-potentials, despite the distribution $\delta'(x)$ in general does not exist. Similarly to the single δ-well potential, beyond the resonance set, the two-sided boundary conditions are of the Dirichlet type: $\psi(\pm 0) = 0$.

On the resonance set $\Sigma = \cup_n \sigma_n$, the explicit expressions for the Λ-matrix (79) and the element (77) become

$$\Lambda|_\Sigma = \begin{pmatrix} \theta_n & 0 \\ \alpha_n & \theta_n^{-1} \end{pmatrix}, \quad (81)$$

where

$$\begin{aligned}
\theta_n &= \frac{\cosh(\sqrt{a_1}\, d_1)}{\cos(\sqrt{|a_2 + b_{1,n}|}\, d_2)} \neq \pm 1,\\
\alpha_n &= \frac{1}{4}\left[\frac{\sqrt{a_1}\, b_2}{|a_2 + b_{1,n}|^{3/2} d_2} - \frac{\sqrt{|a_2 + b_{1,n}|}\, b_{1,n}}{a_1^{3/2} d_1}\right]\\
&\quad \times \sinh(\sqrt{a_1}\, d_1)\sin(\sqrt{|a_2 + b_{1,n}|}\, d_2). \quad (82)
\end{aligned}$$

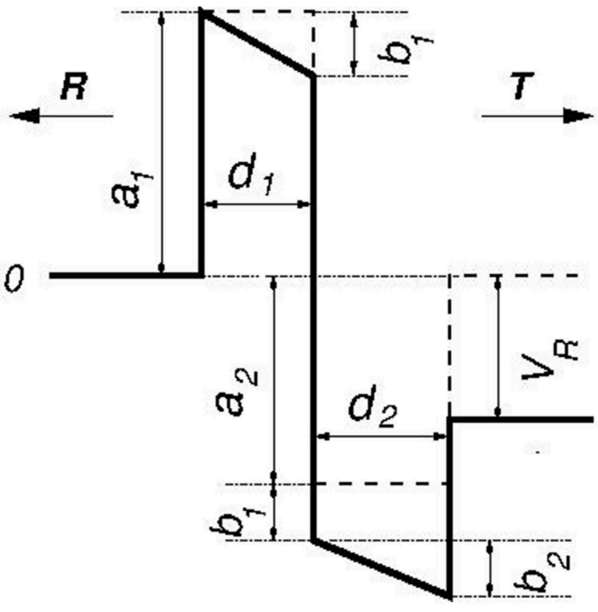

FIGURE 3 | Schematics of tilted (solid line) and piecewise constant (dashed line) barrier-well potential, where notations correspond to Equations (73) and (74) for $N = 2$ and $\varepsilon = 1$. Potential values at layer edges are $V_{1,0} = a_1$, $V_{1,1} = a_1 + b_1$ (barrier, $a_1 > 0$) and $V_{2,1} = a_2 + b_1$, $V_{2,2} = a_2 + b_1 + b_2$ (well, $a_2 < 0$). Polarity is shown positive (left-to-right electron flow, $b_1, b_2 < 0$). Dashed lines show unbiased potential ($b_1 = b_2 = 0$).

The transmission amplitude on the resonance set Σ is

$$\mathcal{T}_n = \frac{4k\,k_{R,n}}{(k\theta_n^{-1} + k_{R,n}\theta_n)^2 + \alpha_n^2}, \tag{83}$$

where $k_{R,n} = \sqrt{k^2 - b_{1,n}}$.

Resonant transmission through a δ-barrier: Let us consider now the two-layered structure in which the potential of one of the layers in the squeezed limit has a δ-like form. We specify this situation by the power parameters $\mu_1 = \nu_1 = 1$ (point $P_{1,1} \in S_0$) for the barrier, and $\mu_2 = 2$ and $\nu_2 = 1$ (point $P_{2,1} \in S_\infty$) for the well. Even in the unbiased case this potential has no distributional limit, however the transmission matrix does exist. Applying the replacement rules (73)-(75) in the asymptotics (67) with $\mu = 1$ yielding the Λ_1-matrix, and in the representation (71) creating the Λ_2-matrix, we obtain the $\varepsilon \to 0$ limit for the elements of the total matrix $\Lambda = \Lambda_2\Lambda_1$ in the form

$$\begin{aligned}
\lambda_{11} &\to \cos(\kappa_2 d_2),\\
\lambda_{12} &\to 0,\\
\lambda_{21} &\to \alpha_1 \cos(\kappa_2 d_2) + c_{1,1}\kappa_2 \sin(\kappa_2 d_2) - \varepsilon^{-1}\kappa_2 \sin(\kappa_2 d_2),\\
\lambda_{22} &\to \cos(\kappa_2 d_2) - \kappa_2 d_1 \sin(\kappa_2 d_2).
\end{aligned} \tag{84}$$

While the first and the second terms in λ_{21} are finite, the third one diverges as $\varepsilon \to 0$. However, it vanishes at the values satisfying the equation $\sin(\kappa_2 d_2) = 0$, i.e., for

$$a_2 + b_{1,n} = -(n\pi/d_2)^2, \tag{85}$$

where the integer $n = n_0, n_0 + 1, \ldots$ with some n_0. These values form the countable resonance set Σ on which the transmission matrix Λ corresponds to the δ-interaction, whereas beyond this set the interaction acts as a fully reflecting wall. The limit transmission matrix is

$$\Lambda|_\Sigma = (-1)^n \begin{pmatrix} 1 & 0 \\ \alpha_n & 1 \end{pmatrix}, \tag{86}$$

where $\alpha_n = \alpha_{1,n} = (a_1 + b_{1,n})/2)d_1$. Note that the effect of the resonant transmission through a δ-barrier keeps to be valid in the unbiased case when $b_1 = b_2 = 0$.

Thus, we have realized the *resonant* δ-interaction, due to the presence of an adjacent well with depth $a_2 < 0$. In the case when the system parameters a_1, a_2, d_1, d_2 are supposed to be fixed, the biased potential b_1 may be considered as a tunable parameter. The transmission is resonant on the set given by (85). The potential at the right edge of the first layer keeps to be positive for all values of b_1 satisfying the inequality $-b_1 < a_1$. Therefore, this is a constraint that limits the resonance set to a finite number of resonances.

The existence of the resonant tunneling through a δ-like barrier can be supported numerically calculating the transmission amplitude $\mathcal{T}$ according to Equations (37) and (34), where the matrix elements are given by Equation (45). For different values of the squeezing parameter ε, the result of these calculations is illustrated by **Figure 4**.

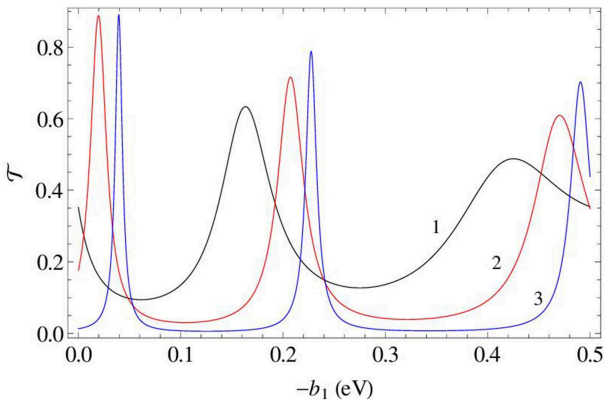

FIGURE 4 | Transmission amplitude $\mathcal{T}$ as a function of bias $-b_1$ plotted for parameter values: $E = 0.1$ eV, $a_1 = 0.5$ eV, $a_2 = -0.1$ eV, $d_1 = 2$ nm, $d_2 = 10$ nm. Computations have been carried out with powers $\mu_1 = \nu_1 = 1$ (point $P_{1,1}$) and $\mu_2 = 2$, $\nu_2 = 1$ (point $P_{2,1}$). Squeezing scenario is displayed for $\varepsilon = 0.5$ (curve 1, black), 0.25 (curve 2, red), and 0.1 (curve 3, blue). Location of all three peaks converges to set $\{-b_{1,n}\}$ defined by Equation (85) with $n = 2, 3, 4$.

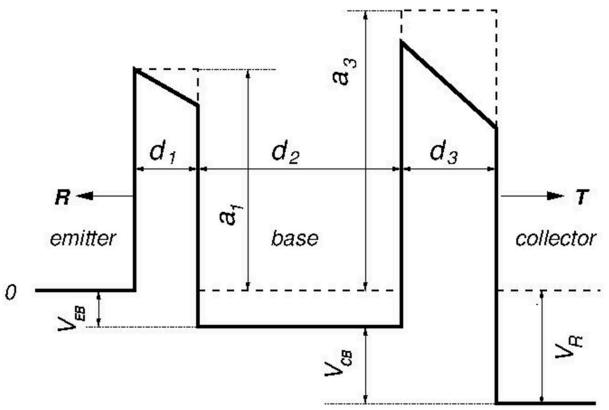

FIGURE 5 | Schematics of typical transistor, where notations correspond to Equations (73) and (74) for $N = 3$ and $\varepsilon = 1$ with replacement: $b_1 \to -V_{EB}$ (emitter-to-base voltage) and $b_3 \to -V_{CB}$ (collector-to-base voltage). Potential values at layer edges are $V_{1,0} = a_1$, $V_{1,1} = a_1 - V_{EB}$ ($a_1 > 0$), $V_{2,1} = V_{2,2} = -V_{EB}$ and $V_{3,2} = a_3 - V_{EB}$, $V_{3,3} = a_3 + V_R$ ($a_3 > 0$). Polarity is shown to be positive (left-to-right electron flow, $V_{EB}, V_{CB} > 0$).

6.2. Modeling of Point Transistors

It is of interest to give an interpretation for a semiconductor transistor in the limit as its dimensions are extremely tiny. This is a three-terminal device [76] described by a tilted double-barrier potential profile as illustrated by **Figure 5**. Here the potential between the barriers is constant depending on the emitter-to-base voltage V_{EB} as a parameter tuned externally. The other external parameter V_{CB} is the collector-to-base voltage being fixed. For the description of this device by a one-point interaction model, we assume that in the zero-thickness limit both the barriers as well as the distance between them tend to the point $x = 0$.

Similarly to the double-layer structure [see the general formula (24)], the transmission matrix for the total system is the product $\Lambda = \Lambda_3\Lambda_2\Lambda_1$, where the matrices Λ_1 and Λ_3 correspond to the barriers and the Λ_2-matrix to the space between the barriers. Setting $b_1 \equiv -V_{EB}$, $b_2 = 0$ and $b_3 \equiv -V_{CB}$, according to (73), we replace: $a \to a_1$ for Λ_1, $a \to -V_{EB}$ ($a_2 = 0$) for Λ_2 and $a \to a_3 - V_{EB}$ for Λ_3. In the case of positive polarity, as shown in the figure, both the voltages are non-negative parameters. Applying next the replacement rules (75) in the terms (68), (69), and (72), we write the following explicit expressions for the matrices Λ_1 and Λ_3:

$$\begin{aligned}
\kappa_1 &= \sqrt{-a_1}\,,\ \kappa_2 = \sqrt{V_{EB}}\,,\ \kappa_3 = \sqrt{V_{EB}-a_3}\,,\\
\alpha_1 &= (a_1 - V_{EB}/2)d_1\,,\ \alpha_3 = (a_3 - V_{EB} - V_{CB}/2)d_3\,,\\
c_{1,1} &= (a_1^2/2)(a_1 - V_{EB})(d_1/V_{EB})^2,\\
c_{1,2} &= (a_1/2)(a_1 - V_{EB})^2(d_1/V_{EB})^2,\\
c_{3,1} &= [(a_3 - V_{EB})^2/2](a_3 - V_{EB} - V_{CB})(d_3/V_{CB})^2,\\
c_{3,2} &= [(a_3 - V_{EB})/2](a_3 - V_{EB} - V_{CB})^2(d_3/V_{CB})^2,\\
g_1 &= -\kappa_1^{-3}(V_{EB}/4d_1),\ g_3 = -\kappa_3^{-3}(V_{CB}/4d_3). \qquad (87)
\end{aligned}$$

The Λ_2-matrix is defined by (48) for $i = 2$, where $k_2 = \kappa_2\varepsilon^{-1}$ and $l_2 = \varepsilon d_2$.

Below we examine the following two zero-thickness limits: (i) $\mu_1 = \mu_3 = \nu_1 = \nu_3 = 1$ (points $P_{1,1}$) and (ii) $\mu_1 = \mu_3 = 2$, $\nu_1 = \nu_3 = 1$ (points $P_{2,1}$).

(i) δ-potential model: The matrix multiplication yields the asymptotic representation in the limit as $\varepsilon \to 0$:

$$\begin{aligned}
&\lambda_{11} \to \cos(\kappa_2 d_2) - \kappa_2 d_3 \sin(\kappa_2 d_2),\\
&\lambda_{12} \to 0,\\
&\lambda_{21} \to (\alpha_1 + \alpha_3)\cos(\kappa_2 d_2) + (c_{1,1} + c_{3,2})\kappa_2 \sin(\kappa_2 d_2) -\\
&\varepsilon^{-1}\kappa_2 \sin(\kappa_2 d_2),\\
&\lambda_{22} \to \cos(\kappa_2 d_2) - \kappa_2 d_1 \sin(\kappa_2 d_2). \qquad (88)
\end{aligned}$$

Here, the element λ_{21} diverges as $\varepsilon \to 0$ and it will be finite if $\sin(\kappa_2 d_2) = 0$, resulting in the resonance set

$$V_{EB,n} = (n\pi/d_2)^2,\ \ n = \overline{1, n_0}\,, \qquad (89)$$

where the integer n_0 depends on the interval of admissible values of the bias potential V_{EB}. This interval is determined by the requirement that the barrier potential values $V_{1,1}$ and $V_{3,3}$ must be positive, leading to the inequalities $0 < V_{EB} < a_1$ and $0 < V_{EB} + V_{CB} < a_3$. Therefore, the potential V_{EB} is allowed to tune within the interval $0 < V_{EB} < \min\{a_1,\, a_3 - V_{CB}\}$.

Thus, the limit transmission matrix is of the form (86) with

$$\alpha_n = \alpha_{1,n} + \alpha_{3,n} = (a_1 - V_{EB,n}/2)d_1 + (a_3 - V_{EB,n} - V_{CB}/2)d_3 > 0. \qquad (90)$$

realizing the δ-potential defined on the resonance set described by Equation (89).

According to the general expressions (37) and (34), the transmission amplitude, being non-zero on this resonance set, is given by the formula (83), where $\theta_n = 1$ and $k_{R,n} = \sqrt{k^2 + V_{EB,n} + V_{CB}}$. The transmission amplitude $\mathcal{T}$ displayed in **Figure 6** illustrates the convergence of the location of the peaks to the roots of Equation (89).

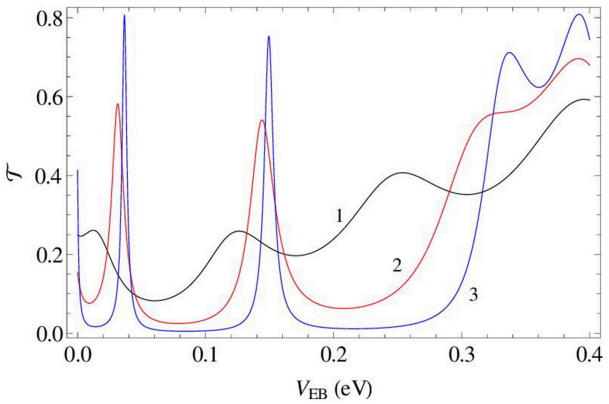

FIGURE 6 | Transmission amplitude $\mathcal{T}$ as a function of emitter-to-base voltage V_{EB} for parameter values: $E = 0.1$ eV, $a_1 = a_3 = 0.5$ eV, $a_2 = 0$, $V_{CB} = 0.2$ eV, $d_1 = d_3 = 2$ nm, $d_2 = 10$ nm. Computations have been carried out with powers $\mu_1 = \nu_1 = \mu_3 = \nu_3 = 1$ (points $P_{1,1}$) and $\mu_2 = 2$, $\nu_2 = 0$. Squeezing scenario is displayed for $\varepsilon = 0.5$ (curve 1, black), 0.25 (curve 2, red), and 0.1 (curve 3, blue). Location of all three peaks approaches set $\{V_{EB,n}\}$ given by Equation (89) with $n = 1, 2, 3$.

(ii) δ′-potential model: The three-lateral device can also be approximated by a δ'-interaction with a bias if we choose for the zero-thickness limit the powers $\mu_1 = \mu_2 = \mu_3 = 2$ and $\nu_1 = \nu_3 = 1$. The multiplication of the matrices yields

$$\begin{aligned}
&\lambda_{11} \to \cos(\kappa_1 d_1)\cos(\kappa_2 d_2)\cos(\kappa_3 d_3)\\
&-(\kappa_1/\kappa_2)\sin(\kappa_1 d_1)\sin(\kappa_2 d_2)\cos(\kappa_3 d_3)\\
&-(\kappa_1/\kappa_3)\sin(\kappa_1 d_1)\cos(\kappa_2 d_2)\sin(\kappa_3 d_3)\\
&-(\kappa_2/\kappa_3)\cos(\kappa_1 d_1)\sin(\kappa_2 d_2)\sin(\kappa_3 d_3),\\
&\lambda_{12} \to 0,\\
&\lambda_{21} \to \kappa_2[g_1 \sin(\kappa_1 d_1)\cos(\kappa_3 d_3)\\
&-g_3 \cos(\kappa_1 d_1)\sin(\kappa_3 d_3)]\sin(\kappa_2 d_2)\\
&+(\kappa_3 g_1 - \kappa_1 g_3)\sin(\kappa_1 d_1)\cos(\kappa_2 d_2)\sin(\kappa_3 d_3)\\
&-\varepsilon^{-1}[\kappa_1 \sin(\kappa_1 d_1)\cos(\kappa_2 d_2)\cos(\kappa_3 d_3)\\
&+\kappa_2 \cos(\kappa_1 d_1)\sin(\kappa_2 d_2)\cos(\kappa_3 d_3)\\
&+\kappa_3 \cos(\kappa_1 d_1)\cos(\kappa_2 d_2)\sin(\kappa_3 d_3)\\
&-(\kappa_1\kappa_3/\kappa_2)\sin(\kappa_1 d_1)\sin(\kappa_2 d_2)\sin(\kappa_3 d_3)],\\
&\lambda_{22} \to \cos(\kappa_1 d_1)\cos(\kappa_2 d_2)\cos(\kappa_3 d_3)\\
&-(\kappa_2/\kappa_1)\sin(\kappa_1 d_1)\sin(\kappa_2 d_2)\cos(\kappa_3 d_3)\\
&-(\kappa_3/\kappa_1)\sin(\kappa_1 d_1)\cos(\kappa_2 d_2)\sin(\kappa_3 d_3)\\
&-(\kappa_3/\kappa_2)\cos(\kappa_1 d_1)\sin(\kappa_2 d_2)\sin(\kappa_3 d_3), \qquad (91)
\end{aligned}$$

where the notations for $\kappa_1, \kappa_2, \kappa_3$, and g_1, g_3 can be found in Equation (87). The arguments of the trigonometric functions are finite and the element λ_{21} diverges as $\varepsilon \to 0$ because of the presence of the factor ε^{-1}. Therefore, the only opportunity to define properly a point interaction is a full cancelation of all the

terms at this factor, so that λ_{21} becomes finite. As a result, this cancelation yields the following equation:

$$\frac{\kappa_1\kappa_3}{\kappa_2}\prod_{i=1}^{3}\tan(\kappa_i d_i)=\sum_{i=1}^{3}\kappa_i\tan(\kappa_i d_i). \tag{92}$$

Using the resonance equation (92), we derive that the pair $\{\lambda_{11},\lambda_{22}\}$ admits the following sixteen representations:

$$\{\lambda_{11},\lambda_{22}\}=\{I_1,I_2,J_1^{-1},J_2^{-1}\}\times\{I_1^{-1},I_2^{-1},J_1,J_2\}, \tag{93}$$

where

$$\begin{aligned}
I_1 &= \frac{\cos(\kappa_1 d_1)\cos(\kappa_2 d_2)-(\kappa_1/\kappa_2)\sin(\kappa_1 d_1)\sin(\kappa_2 d_2)}{\cos(\kappa_3 d_3)},\\
I_2 &= -\frac{\kappa_1\sin(\kappa_1 d_1)\cos(\kappa_2 d_2)+\kappa_2\cos(\kappa_1 d_1)\sin(\kappa_2 d_2)}{\kappa_3\sin(\kappa_3 d_3)},\\
J_1 &= \frac{\cos(\kappa_2 d_2)\cos(\kappa_3 d_3)-(\kappa_3/\kappa_2)\sin(\kappa_2 d_2)\sin(\kappa_3 d_3)}{\cos(\kappa_1 d_1)},\\
J_2 &= -\frac{\kappa_2\sin(\kappa_2 d_2)\cos(\kappa_3 d_3)+\kappa_3\cos(\kappa_2 d_2)\sin(\kappa_3 d_3)}{\kappa_1\sin(\kappa_1 d_1)}.
\end{aligned} \tag{94}$$

These representations follow from the equations $I_1 = I_2$, $J_1 = J_2$, and $I_1 J_1 = 1$, which can be checked using the condition (92). As a result, we have $|\Lambda| = \lambda_{11}\lambda_{22} = 1$ if Equation (92) is fulfilled.

Equation (92) can be rewritten in the explicit form as follows

$$\begin{aligned}
&\sqrt{a_1/V_{EB}}\,\tanh(\sqrt{a_1}\,d_1)+\sqrt{a_3/V_{EB}-1}\,\tanh(\sqrt{a_3-V_{EB}}\,d_3)\\
&=\left[1-\sqrt{a_1/V_{EB}}\,\sqrt{a_3/V_{EB}-1}\,\tanh(\sqrt{a_1}\,d_1)\tanh(\sqrt{a_3-V_{EB}}\,d_3)\right]\\
&\times\tan(\sqrt{V_{EB}}\,d_2).
\end{aligned} \tag{95}$$

This form shows the existence of the roots forming a resonance set $\Sigma = \{V_{EB,n}\}$. Inserting next these roots into Equation (94), one can get the discrete values of the diagonal elements $\lambda_{11,n}$ and $\lambda_{22,n}$ of the matrix set $\Lambda|_\Sigma$. One can write then $\theta_n := \lambda_{11,n} = \lambda_{22,n}^{-1} = I_{1,n} = I_{2,n} = J_{1,n}^{-1} = J_{2,n}^{-1}$. Finally, one can represent the off-diagonal element $\lambda_{21,n} = \alpha_n$ as

$$\begin{aligned}
\alpha_n &= a_1^{-3/2}(V_{EB,n}/4d_1)\sinh(\sqrt{a_1}\,d_1)\\
&\times[\sqrt{V_{EB,n}}\cosh(\sqrt{a_3-V_{EB,n}}\,d_3)\sin(\sqrt{V_{EB,n}}\,d_2)\\
&-\sqrt{a_3-V_{EB,n}}\sinh(\sqrt{a_3-V_{EB,n}}\,d_3)\cos(\sqrt{V_{EB,n}}\,d_2)]\\
&-(a_3-V_{EB,n})^{-3/2}(V_{CB}/4d_3)\sinh(\sqrt{a_3-V_{EB,n}}\,d_3)\\
&\times[\sqrt{V_{EB,n}}\cosh(\sqrt{a_1}\,d_1)\sin(\sqrt{V_{EB,n}}\,d_2)\\
&-\sqrt{a_1}\sinh(\sqrt{a_1}\,d_1)\cos(\sqrt{V_{EB,n}}\,d_2)].
\end{aligned} \tag{96}$$

Similarly to the double-layer structure with the limit transmission matrix (81), we refer this one-point interaction to as the δ'-potential because $\lambda_{11,n}, \lambda_{22,n} \neq 1$. The transmission amplitude is given by the same formula (83) in which $\theta_n = \lambda_{11,n}$ and $\alpha_n = \lambda_{21,n}$ is given by the expression (96).

7. CONCLUDING REMARKS

In the present work we addressed the family of point interactions as the zero-thickness limit of heterostructures composed of several layers. The latter have energy diagrams stemming from tilted linear potentials that arise as a result of the application of external electric fields. The analysis starts from the solution of the one-dimensional stationary Schrödinger equation for the structure with finite size using the transfer matrix approach. Within this approach, we find the transmission matrices for each layer; their product quantifies the penetration amplitude of electrons through the whole system. In order to realize point interactions we introduce a squeezing parameter $\varepsilon > 0$ in the structural parameters of the system (layer width, potentials at layer edges, etc.) leading to shrinking the thickness of the system as $\varepsilon \to 0$. In this limit the potential values at the interfaces of layers must go to infinity if we wish to create a point interaction in the squeezed limit. At $\varepsilon = 1$, the structural parameters correspond to realistic values of the device.

One of interesting features discovered in the previous publications [17, 43–45, 48, 49, 51] is the appearance of electron tunneling through one-point barriers that occurs at some discrete values of system parameters, whereas beyond these values the system behaves as a fully reflecting wall. The origin of this phenomenon is an oscillating behavior of particle transmission. Surprisingly, as the system shrinks to a point, the oscillating regular function that describes the transmission amplitude, converges pointwise to the function with non-zero finite values only at some discrete points in the space of system parameters, whereas beyond this (resonance) set, the system acts a fully reflecting wall (see, e.g., **Figure 1** in Zolotaryuk and Zolotaryuk [17]). In other words, the maxima of the oscillating amplitude correspond in the squeezing limit to the set of extremely sharp peaks. On the other hand, in many devices the oscillating behavior of transmitted particles appears as a function of tuning some controllable (not system) parameters. For instance, in the typical point transistor, an emitter-to-base voltage may be served as such a parameter. Indeed, the electron flow across this device is an oscillating function of this voltage. In this regard, it is of interest to construct the point interactions with a resonance set controllable by parameters applied externally and this is the main goal of the present paper.

In conclusion, in the present paper we have tried to develop the general approach on how to realize the point interactions as a zero-thickness limit of structures composed of an arbitrary number of layers with biased potentials. This approach is specified by the examples describing one layer, the double- and three-layer systems. The piecewise linear potentials are not required to have any distributional limit as $\varepsilon \to 0$. Despite this, the $\varepsilon \to 0$ limit of the transmission matrices has been shown to exist enable us to compute analytically the transmission amplitude. The most interesting phenomenon discussed in the present paper is the appearance of the resonant transmission through a δ-like barrier in the presence

of an adjacent well. The origin of this effect emerges from the fact that the particle transmission across a well has an oscillating behavior. This behavior keeps to be of the same nature after tunneling through a barrier. Therefore, in the squeezed limit this oscillating transforms into the function with non-zero values only at discrete points, whereas on the intervals between these points, this function converges pointwise to zero resulting in blocking the tunneling trough the barrier.

DATA AVAILABILITY

The raw data supporting the conclusions of this manuscript will be made available by the authors, without undue reservation, to any qualified researcher.

AUTHOR CONTRIBUTIONS

AZ, GT, and YZ contributed equally in all stages of this work. YZ contributed to calculations of transmission amplitudes.

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A Distributional Approach for the One-Dimensional Hydrogen Atom

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We consider the one-dimensional Hydrogen atom, with the Coulomb interaction $V(x) = \frac{\gamma}{|x|}$ ($\gamma < 0$), and use Schwartz's theory of distributions to address the non-integrable singularity at the origin. This singularity renders the interaction term $V(x)\psi(x)$ in the Schrödinger's equation, where $\psi(x)$ is the wave function, an ill-defined product in the ordinary sense. We replace this ill-defined product by a well-defined interaction *distribution*, $S[\psi, V](x)$, and by imposing that it should satisfy some fundamental mathematical and physical requirements, we show that this distribution is defined up to a 4-parameter family of contact interactions, in agreement with the method of self-adjoint extensions. By requiring that the interaction distribution be invariant under parity, we further restrict the 4-parameter family of interactions to the subfamily of all the parity invariant Coulomb interactions. Finally, we present a *systematic* study of the bound states within this subfamily, addressing the frequently debated issues of the multiplicity and parity of the bound states, and the boundedness of the ground state energy.

Keywords: one-dimensional quantum mechanics, singular interactions, contact interactions, Coulomb interaction, one-dimensional Hydrogen atom, Schwartz's distribution theory, parity invariance

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1. INTRODUCTION

The one-dimensional (1D) hydrogen atom, with a Coulomb-like interaction[1], is defined by the Hamiltonian (throughout this paper we use Rydberg atomic units $\frac{\hbar}{2m} = 1$)

$$H = -\frac{d^2}{dx^2} + \frac{\gamma}{|x|}, \qquad x \neq 0, \quad \gamma < 0, \tag{1}$$

and it has been a source of considerable interest since the paper by Loudon [1], who investigated this problem due to its relevance for the physics of excitons in strong magnetic fields. The 1D Coulomb potential finds applications in several fields, such as the quasi one-dimensional hydrogen atom in astrophysical systems with very strong magnetic fields [2], in quantum wires and carbon nanotubes (see, e.g., [3–5] and references therein), *etc.*—for a recent review of the applications of the 1D Coulomb interaction see Loudon [6].

Despite its many applications and deceptive simplicity, the 1D hydrogen atom has been a source of great controversy in the literature. This is due to the fact that the 1D Coulomb potential has a non-integrable singularity at the origin, rendering its mathematical treatment non-trivial. In

[1]It should be noticed that the potential in Equation (1), $V(x) = \frac{\gamma}{|x|}$, is not the solution of the 1D Maxwell's equations for a point source, see for example [7, 8]. Nevertheless, we follow the practice in the literature and call it the 1D Coulomb potential.

particular, the singularity at the origin makes it unclear what are the boundary conditions (b.c.) to be used there and, consequently, whether the potential is impenetrable or not at the singularity (see, e.g., [7]). This singularity also obscures the properties of the system under parity transformations, since the behavior of $V(x) = \frac{\gamma}{|x|}$ on $\mathbb{R}\backslash\{0\}$ is not sufficient to ensure that the system is parity invariant (see section 3 for further details).

Several treatments, including Loudon's [1], regularize the potential by introducing a small cutoff a via $V(x) = \gamma/(|x| + a)$, and taking the limit $a \to 0$ at the end. This regularization procedure has led to conflicting results in which concerns the degeneracy or not of the spectrum, the existence of even wave functions and whether the associated spectrum is continuous or discrete, and the stability of the model (unboundedness of the ground state energy from below, in the $a \to 0$ limit) [1, 6, 9, 10]. This is, perhaps, unsurprising, since regularization procedures need to be employed with great care and often need additional input, such as symmetry, to yield meaningful results, as is well-known in quantum field theory [11] or in the study of chemical indices [12, 13]—see [14, 15] for rigorous treatments of the regularized 1D Coulomb potential, and [16] for a general treatment of regularized Sturm-Liouville operators.

Many other approaches, such as the use of generalized Laplace transform [17], Fourier transform [18], superpotentials [8], among others [19–23], have also been employed in the solution of the 1D hydrogen atom. Still, these either have not addressed or have not been able to unequivocally resolve all the issues above mentioned. Recognizing that the Hamiltonian corresponding to (1) is symmetric, but not self-adjoint, has led to the application of the rigorous theory of self-adjoint extensions (SAE) of symmetric operators to this problem by several authors [7, 24–27], who have shown that the Hamiltonian (1) is not essentially self-adjoint and, therefore, does not have a unique self-adjoint extension [28]. In fact, it has been shown in the SAE approach that this Hamiltonian admits a four-parameter family of extensions [7, 29].

Despite SAE's rigorous and unequivocal results, confusion still persists in the literature, particularly concerning the parity of the solutions and the boundedness or not of the ground state energy. In addition, although the method of SAE clarifies the possible extensions of the Hamiltonian, it cannot decide which extension (or b.c.) is the physically sensible one. Thus, a more physically appealing, albeit still rigorous, alternative method is certainly desirable and may help to shed light on some of the open problems remaining in the field. With this in mind, in section 2 we revisit the 1D Coulomb interaction and address the singularity using the Schwartz's theory of distributions, thus generalizing the method recently developed for 1D contact interactions [30] (also see [31]) to include long-range singular interactions. In this approach we deal with the non-integrable singularity of the potential at the origin by replacing the (generally) ill defined product $V(x)\psi(x)$ in the Schrödinger equation by a well-defined interaction distribution $S[\psi, V]$, to be determined from fundamental mathematical and physical requirements. Such requirements are imposed on the interaction distribution in order that fundamental postulates of quantum mechanics, such as the superposition principle and probability conservation, be satisfied also in the singular case. The interaction distribution is, essentially, a *distributional* regularization of the (ill-defined) term $V(x)\psi(x)$ and, by a general result of the distribution theory [32], it is determined only up to a sum of contact interactions at the singularity (that is, the Dirac delta and it's derivatives). We show that the requirements imposed on the interaction distribution reduce the contact terms to a four parameter family of point interactions, thus agreeing with the SAE results [7, 29]. It should be noticed that Kurasov used distributional methods to address singular potentials, including the 1D Coulomb potential [24]. However, Kurasov uses distribution theory in the context of the self-adjoint operator theory, in order to obtain the particular Friedrichs extension of the symmetric operator (1), also see [25, 33, 34]. Our approach is fundamentally different in which here the only requirements are from within the distribution theory and simple physical requirements from quantum theory. In addition, an explicit general form for the interaction distribution $S[\psi, V]$ is constructed, including all interactions of the four-parameter family of contact interactions, a feature that renders the distributional approach particularly suitable for symmetry analyses [30, 31].

We argue that, given the parity invariance of the original Coulomb potential on $\mathbb{R}\backslash\{0\}$, it is natural to impose the same property for the interaction distribution—we, again, stress that the parity invariance of the potential $V(x)$ on $\mathbb{R}\backslash\{0\}$ is not sufficient to ensure that the *interaction*, defined on the entire $\mathbb{R}$, is invariant: the behavior of the contact interactions must also be taken into account. Thus, in section 3 we show that requiring parity invariance further reduces the allowed interactions to either a two-parameter interaction (permeable origin) or an one-parameter interaction (impermeable origin) [30]. We then present, in section 4, a systematic study of the bound states for the subfamily of *all* parity invariant interactions, addressing questions that are at the origin of the controversies about the 1D hydrogen atom in the literature, such as the multiplicities of bound state energies, the parity of the corresponding eigenfunctions and the boundedness of the ground state (see [6, 7, 26] and references therein)—as far as we know, such a systematic investigation, including all possible parity invariant b.c., is missing in the literature and it may help to clarify the controversies mentioned above. The results are discussed in section 5 and two appendices, on essentials of distribution theory and the solutions of the Whittaker equation, are included for convenience.

2. A DISTRIBUTIONAL APPROACH TO THE 1D HYDROGEN ATOM INTERACTION

The time independent 1D Schrödinger equation

$$-\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x) \tag{2}$$

introduces the interaction of a quantum particle with an external potential $V(x)$ via the product $V(x)\psi(x)$, which is well-defined for potentials described by regular distributions. However, for

singular potentials, such as the (attractive) 1D Coulomb potential

$$V(x) = \frac{\gamma}{|x|}, \qquad x \neq 0, \quad \gamma < 0, \tag{3}$$

the product $V(x)\psi(x)$ is ill-defined, due to the singularity of the potential at the origin. We will address this difficulty by considering the Schrödinger equation in the distributional sense, that is, every term in Equation (2) must correspond to a distribution. This requires particular attention to the product term $V(x)\psi(x)$, not only due to the singularity of the 1D Coulomb potential, but also because the *naive* product of two distributions is not necessarily a well-defined distribution.

2.1. The 1D Coulomb Potential as a Distribution

The 1D Coulomb potential, Equation (3), has a (Lebesgue) non-integrable singularity at the origin (its integral diverges logarithmicaly near the origin). As a consequence, it *does not* define a *regular* distribution[2] on any open interval including the origin. However, it defines a regular distribution on any open interval which does not include the origin, such as $\mathbb{R}\backslash\{0\}$. Any distribution defined on the entire real line and which coincides with $V(x)$ on $\mathbb{R}\backslash\{0\}$ [that is, a distributional regularization of $V(x)$] will necessarily be *singular*, and it *will not be unique*. In fact, the difference between any two distributions satisfying this requirement [i.e., between two *distributional* regularizations of $V(x)$] is a distribution concentrated at the origin, hence given by a linear combination of the delta distribution and its derivatives up to (and including) the greatest order of the two distributions (see the Theorem in **Appendix 1**).

Let r_c be the order of any distribution $V_c(x)$ defined on the entire real line and coinciding with $V(x) = \frac{\gamma}{|x|}$ on $\mathbb{R}\backslash\{0\}$. Then, the minimum possible value for r_c is zero. To see this, observe that on $\mathbb{R}\backslash\{0\}$ any primitive of $V_c(x)$ must have the general form $V_c^{(-1)}(x) = \gamma\,\mathrm{sgn}(x)\log|x| + c_1 + c_2\theta(x)$, with c_1 and c_2 arbitrary constants and θ the Heaviside theta distribution[3] (see **Appendix 1** for the notation). The function $V_c^{(-1)}(x)$ diverges logarithmically as $x \to 0^{\pm}$, but it is *integrable around the origin* and, thus, it must be the derivative of a continuous (but not differentiable at $x = 0$) function. It follows that $V_c^{(-1)} = W^{(1)}(x)$, with

$$W(x) = \gamma|x|(\log|x| - 1) + c_1 x + c_2 t(x) + c_3, \tag{4}$$

where $t(x) = x\theta(x)$ is a continuous function [a primitive of $\theta(x)$] and c_3 is another arbitrary constant. We have, for instance, that $W(0) \equiv \lim_{x\to 0}\gamma|x|(\log|x| - 1) + c_3 = c_3$. Therefore, we have found a continuous function $W(x)$, not differentiable at the origin, whose second distributional derivative is a distribution $V_c(x)$ which coincides with $\frac{\gamma}{|x|}$ on $\mathbb{R}\backslash\{0\}$. Hence, we conclude that $W(x)$ has order -2 and, consequently, $V_c(x) = W^{(2)}(x)$ has order zero (see **Appendix 1**). Any other distribution coinciding with $\frac{\gamma}{|x|}$ on $\mathbb{R}\backslash\{0\}$, and also having order zero, must differ from $V_c(x)$ only by a multiple of the delta distribution (see the Theorem in **Appendix 1**).

2.2. The Interaction Distribution

Let us now, following the approach introduced in Calçada et al. [30], substitute the ill-defined product $V(x)\psi(x)$ in the time independent Schrödinger equation by a well-defined distribution $S[\psi, V]$[4]. Then, the distributional Schrödinger equation takes the form:

$$\psi'' + E\psi = S[\psi, V]. \tag{5}$$

The *interaction distribution* $S[\psi, V]$ must be determined from fundamental mathematical and physical requirements, namely,

R1. The distribution $S[\psi, V]$, defined on the entire real line, must coincide with $V(x)\psi(x)$ on $\mathbb{R}\backslash\{0\}$;
R2. The distribution $S[\psi, V]$ must depend linearly on the wave function ψ and its derivative.
R3. The wave function must correspond to a regular distribution (i.e., to a locally integrable function in the Lebesgue sense) in any interval around the origin. Thus, its order, r_ψ, must be bounded from above by $r_\psi \leq -1$.
R4. The probability flux must be conserved across the origin.

The reasons why any well-defined system needs to satisfy these requirements are as follows. **R1** is a purely mathematical necessity from the definition of a distributional regularization (and it is self-evident). **R2** is necessary for the superposition principle to hold and in order for the dynamics to be given by Schrödinger's equation for *local* interactions. **R3** is necessary (although not sufficient) to obtain square integrable wave functions around the origin—both **R3** and **R4** are necessary requirements of the probabilistic interpretation of quantum mechanics. Taken together, **R1**–**R4** are equivalent to require self-adjointness of the Hamiltonian (see [28] for requirements similar to **R3** and **R4**, notice that there **R1** and **R2** are automatically satisfied).

Equation (5), with requirement **R1**, applied to the 1D Coulomb interaction, implies that

$$\begin{aligned} \psi'' + E\psi \;&=\; S[\psi, V] = \frac{\gamma}{|x|}\psi, \\ \text{for} \quad x \in \mathbb{R}\backslash\{0\} \;&=\; (-\infty, 0) \cup (0, +\infty)\,. \end{aligned} \tag{6}$$

The general solution for this equation is presented in the **Appendix 2**, in terms of the well-known Whittaker's functions. In what follows, an important property of the solution there presented is the fact that $\psi(x)$ has finite lateral limits $\psi(0^{\pm})$ when $x \to 0^{\pm}$ [see Equation (A6)].

Following the ideas of the previous subsection, we need to find a (ordinary) primitive of the term $\frac{\gamma}{|x|}\psi$, defined on $\mathbb{R}\backslash\{0\}$. It is not difficult to see that, by conveniently choosing the integration constants, we can obtain a primitive in the form of the following

[2]For a definition of the main terms of distribution theory used in this work refer to the **Appendix 1**.

[3]Notice that it is possible to have different arbitrary constants on opposite sides of the origin.

[4]The notation $S[\psi, V]$ is due to the functional dependence on $V(x)$ and $\psi(x)$.

ordinary function[5]

$$G[\psi, V](x) = \gamma \left\{ \psi(x)\,\mathrm{sgn}(x) \ln|x| - \psi'(x)|x| \left(\ln|x| - 1\right) - \int_0^x \psi(t)\,(|t|E - \gamma)\left(\ln|t| - 1\right) dt \right\}, \quad (7)$$

where $\mathrm{sgn}(x) = \theta(x) - \theta(-x)$ stands for the sign function. It can be easily checked that the (ordinary) derivative of $G[\psi, V](x)$ coincides with the ordinary function $\frac{\gamma}{|x|}\psi$ on $\mathbb{R}\backslash\{0\}$, as desired.

It is important to notice that the function $G[\psi, V](x)$ is *locally integrable* and, thus, *defines a distribution over the entire real line*. To demonstrate this, it is enough to check the integrability in any finite interval containing the origin: the first term within the brackets in (7) is locally integrable because $\psi(x)$ is bounded (see **Appendix 2**) and $\ln|x|$ is integrable; the third term (the integral) defines a continuous function for all x, since the integrand is an integrable function, by the same reason of the first term; finally, the middle term is also integrable, since, for any fixed $R > 0$ and arbitrary $\eta > 0$,

$$\int_\eta^R \psi'(x)\,|x|\left(\ln|x| - 1\right) dx = |x|\left(\ln|x| - 1\right)\psi(x)\Big|_\eta^R - \int_\eta^R \psi(x)\ln|x|\,dx,$$

and both terms in the r.h.s of this equation have well-defined limits when $\eta \to 0^+$. The same holds for the integral $\int_{-R}^{-\eta} \psi'(x)\,|x|\left(\ln|x| - 1\right) dx$.

The fact that $G[\psi, V](x)$ defines a regular distribution on the entire real axis implies that its order is $r_G \leq -1$. As a consequence, its *distributional derivative* $G'[\psi, V](x) \equiv S_0[\psi, V](x)$ is defined over the entire real axis, has order ≤ 0 and, as mentioned above, coincides with the product $\frac{\gamma}{|x|}\psi(x)$ when restricted to the region $\mathbb{R}\backslash\{0\}$. Any other distribution $S[\psi, V](x)$ satisfying **R1** must differ from $S_0[\psi, V](x)$ only by a distribution concentrated at the origin (a contact interaction) and, from the Theorem on **Appendix 1**, we have that

$$S[\psi, V](x) = S_0[\psi, V](x) + \sum_{n=0}^{r} c_n[\psi, V]\delta^{(n)}(x), \quad (8)$$

where the (complex) coefficients $c_n[\psi, V]$ must be linear functionals of $\psi(x)$ and its derivative, to satisfy requirement **R2**. From **R3** and the fact that indefinite integration (taking the primitive) decreases the order by one (see **Appendix 1**), the order of $S[\psi, V](x)$, r_s, must be at most $r_s = +1$, since it follows from Equation (5) that the distribution $S[\psi, V](x)$ must have the same order as $\psi''(x)$ (the orders of the δ and δ' are 0 and $+1$, respectively [32]). Therefore, requirements **R1**–**R3** imply that the distributional Schrödinger equation, Equation (5), with the most general interaction distribution $S[\psi, V](x)$, can be written as

$$\psi''(x) + E\,\psi(x) = S_0[\psi, V](x) + c_0[\psi, V]\,\delta(x) + c_1[\psi, V]\,\delta'(x), \quad (9)$$

with $S_0[\psi, V](x) = G'[\psi, V](x)$ and $G[\psi, V](x)$ given by the regular distribution defined by Equation (7). In the above equation the only undetermined quantities are the (functional) coefficients $c_0[\psi, V]$ and $c_1[\psi, V]$, which determine the contact term. Below we show that these coefficients are associated to the b.c. that the wave function and its derivative must satisfy around the origin and, thus, requirement **R4** will restrict the possible choices for them. To this purpose, by taking a primitive of (9), we obtain

$$\left[\psi'(x) - G[\psi, V](x)\right] - c_0[\psi, V]\,\theta(x) - c_1[\psi, V]\,\delta(x) = -E\,\psi^{(-1)}(x) + c_2, \quad (10)$$

with c_2 an arbitrary constant. The distribution on the r.h.s of (10) is a continuous function, since its order is -2.

The lateral and point limits of a singular distribution can be defined (if they exist) even at the singular point [35, 36]. In particular, the lateral limits of the δ-distribution are zero, as follows directly from the fact that the δ vanishes in the open intervals $(-\infty, -\epsilon)$ and $(+\epsilon, +\infty)$ for any $\epsilon > 0$ (see [37], p. 64). Hence, it follows from (10) that the lateral limits of $\left[\psi'(x) - G[\psi, V](x)\right]$ exist and are given by

$$\left[\psi' - G\right]_+ = c_0[\psi, V] - E\,\psi^{(-1)}(0) + c_2;$$
$$\left[\psi' - G\right]_- = -E\,\psi^{(-1)}(0) + c_2,$$

where we used the shorthand notation $\left[\psi' - G\right]_{0^\pm} \equiv \lim_{x\to 0^\pm}\left\{\psi'(x) - G[\psi, V](x)\right\}$. Subtracting these equations we obtain

$$\left[\psi' - G\right]_{0^+} - \left[\psi' - G\right]_{0^-} = c_0[\psi, V], \quad (11)$$

On the other hand, from Equation (7) we obtain that

$$\left[\psi' - G\right]_{0^\pm} = \tilde{\phi}(0^\pm) \equiv \lim_{x\to 0^\pm} \tilde{\phi}(x),$$

where $\tilde{\phi}(x)$ is defined as (see also [7])

$$\tilde{\phi}(x) \equiv \psi'(x) - \mathrm{sgn}(x)\,\gamma\,\psi(x)\,\ln|x|. \quad (12)$$

Thus, the boundary condition (11) can be rewritten as (see [15, 25] for alternative proofs)

$$\tilde{\phi}\left(0^+\right) - \tilde{\phi}\left(0^-\right) = c_0[\psi, V]. \quad (13)$$

Now, by taking a primitive of Equation (10) we obtain, after some rearrangement,

$$\psi(x) - c_1[\psi, V]\,\theta(x) = G^{(-1)}[\psi, V](x) + c_0[\psi, V]\,T(x) - E\psi^{(-2)}(x) + c_2\,x + c_3,$$

[5]The ordinary function $G[\psi, V](x)$, defined on $\mathbb{R}\backslash\{0\}$, can be obtained by following a simple procedure. For $x > 0$, one may start by taking the following primitive of $\frac{\gamma\psi}{|x|}$

$$\int_1^x \frac{\gamma\psi}{|x|}\,dx, \quad x > 0.$$

After integrating twice by parts and using the Schrödinger Equation (6) to rewrite the integrand resulting from the last integration by parts, one finds a primitive defined on $x > 0$. A primitive defined on $x < 0$ may be obtained in a similar way, by replacing the lower limit in the above integral by -1 and repeating the process. Finally, the function $G[\psi, V](x)$ can be obtained from these two primitives, found on each side of the origin, by choosing suitable arbitrary constants.

where $T(x) = \theta^{(-1)}(x) = x\theta(x)$ and c_3 is another arbitrary constant. The r.h.s. of the above equation is a continuous function ($G^{(-1)}[\psi, V](x)$ is a continuous distribution, since it is a primitive of a regular distribution) and, thus, both sides of the equation have well-defined lateral limits when $x \to 0^{\pm}$. Taking the lateral limits and subtracting the corresponding equations we obtain the second boundary condition

$$\psi\left(0^{+}\right) - \psi\left(0^{-}\right) = c_1[\psi, V]. \tag{14}$$

Equations (13,14) give the b.c. satisfied by the wave function and its derivative around the origin in terms of the yet undefined coefficients $c_0[\psi, V]$ and $c_1[\psi, V]$ [which are, in fact, complex-valued linear functionals of $\psi(x)$ and $\psi'(x)$]. Hence, once specified, these coefficients will completely determine the interaction.

Let us now use the requirement **R4**, taking into account the b.c. (13) and (14), to restrict the possibilities for $c_1[\psi, V]$ and $c_2[\psi, V]$. First, notice that on $\mathbb{R}\backslash\{0\}$ the probability current can be conveniently rewritten in terms of $\tilde{\phi}(x)$ as

$$\begin{aligned} j(x) &= -i\left[\psi^*(x)\psi'(x) - \psi(x)\psi'^*(x)\right] \\ &= -i\left[\psi^*(x)\tilde{\phi}(x) - \psi(x)\tilde{\phi}^*(x)\right], \end{aligned} \tag{15}$$

which has well-defined lateral limits around the origin. Probability current conservation now reads $j\left(0^{+}\right) = j\left(0^{-}\right)$ and it may establish (when the current does not vanish) a connection between the values of $\psi(x)$ and $\tilde{\phi}(x)$ on both sides of the origin. This, together with the b.c. (13) and (14), allows us to determine the most general form for $c_0[\psi, V]$ and $c_1[\psi, V]$. The procedure to find these coefficients is identical to that followed in reference [30], and all of the Equations (9–28) from Calçada et al. [30] apply to the current system by replacing $\psi'\left(0^{\pm}\right) \to \tilde{\phi}\left(0^{\pm}\right)$. Thus, below we just summarize the results.

Permeable Interactions. In this case the wave function and its derivative [via $\tilde{\phi}(x)$] on both sides of the origin are connected (hence, the origin is *permeable*). These *non-separated* interactions [30, 38] are characterized by four parameters, and the interaction distribution $S[\psi, V](x)$, in Equation (9), is given by:

$$S[\psi, V](x) = S_0[\psi, V](x) + c_0[\psi, V]\,\delta(x) + c_1[\psi, V]\,\delta'(x), \tag{16}$$

$$c_0[\psi, V] = \left[c\,\mathrm{e}^{i\varphi}\psi\left(0^{-}\right) + \left(d\,\mathrm{e}^{i\varphi} - 1\right)\tilde{\phi}\left(0^{-}\right)\right], \tag{17}$$

$$c_1[\psi, V] = \left[\left(a\,\mathrm{e}^{i\varphi} - 1\right)\psi\left(0^{-}\right) + b\,\mathrm{e}^{i\varphi}\tilde{\phi}\left(0^{-}\right)\right], \tag{18}$$

where $a, b, c, d \in \mathbb{R}$, $ad - bc = 1$ and $\varphi \in [0, \pi)$. The b.c. can be written in the matrix form as:

$$\Phi\left(0^{+}\right) = \Lambda\,\Phi\left(0^{-}\right), \quad \Phi\left(0^{\pm}\right) = \begin{bmatrix} \psi\left(0^{\pm}\right) \\ \tilde{\phi}\left(0^{\pm}\right) \end{bmatrix}, \quad \Lambda = \mathrm{e}^{i\varphi}\begin{bmatrix} a & b \\ c & d \end{bmatrix}. \tag{19}$$

Alternatively, the expression (16) can be rewritten in terms of $\psi\left(0^{+}\right)$, $\tilde{\phi}\left(0^{+}\right)$ by inverting the relations (19), resulting in Calçada et al. [30]:

$$c_0[\psi, V] = \left[c\,\mathrm{e}^{-i\varphi}\psi\left(0^{+}\right) - \left(a\,\mathrm{e}^{-i\varphi} - 1\right)\tilde{\phi}\left(0^{+}\right)\right], \tag{20}$$

$$c_1[\psi, V] = -\left[\left(d\,\mathrm{e}^{-i\varphi} - 1\right)\psi\left(0^{+}\right) - b\,\mathrm{e}^{-i\varphi}\tilde{\phi}\left(0^{+}\right)\right]. \tag{21}$$

Impermeable Interactions. In this case we have a *separated* two-parameter family of interactions [30, 38], characterized by $j\left(0^{-}\right) = j\left(0^{+}\right) = 0$, such that $\psi(x)$ and $\tilde{\phi}(x)$ on both sides of the origin are not connected (hence, an impermeable origin). The associated b.c. are given by

$$\tilde{\phi}\left(0^{\pm}\right) = h^{\pm}\psi\left(0^{\pm}\right), \tag{22}$$

where $h^{\pm} \in \mathbb{R}\cup\{+\infty\}$, with he interaction distribution assuming the form[6]

$$S[\psi, V](x) = S_0[\psi, V](x) + c_0[\psi, V]\,\delta(x) + c_1[\psi, V]\,\delta'(x), \tag{23}$$

$$c_0[\psi, V] = \left[h^{+}\psi\left(0^{+}\right) - h^{-}\psi\left(0^{-}\right)\right] = \left[\tilde{\phi}\left(0^{+}\right) - \tilde{\phi}\left(0^{-}\right)\right], \tag{24}$$

$$c_1[\psi, V] = \left[\psi\left(0^{+}\right) - \psi\left(0^{-}\right)\right] = \left[\frac{1}{h^{+}}\tilde{\phi}\left(0^{+}\right) - \frac{1}{h^{-}}\tilde{\phi}\left(0^{-}\right)\right]. \tag{25}$$

3. SYMMETRY: PARITY INVARIANCE

As we have seen in the previous section, the fundamental requirements **R1**-**R4**, which must be satisfied by all interactions, restrict the possible choices for the coefficients $c_0[\psi, V]$ and $c_1[\psi, V]$ to either a family of interactions with four independent parameters (in the permeable case) or to a family of interactions with two independent parameters (in the impermeable case). To further restrict the possible interactions we need to impose additional, *physical*, requirements.

A natural way to select subfamilies of interactions is by requiring that the underlying symmetries of the potential be maintained in the distributional theory. Hence, given that the Coulomb *potential* (3) is invariant under parity [i.e., an even function], we will require that the distribution interaction $S[\psi, V](x)$ introduced in (9) also be invariant under parity transformation. It should be noticed that, despite the fact that Coulomb's potential is an even function under parity, $S[\psi, V](x)$ *does not* necessarily have a definite parity. It is only for *particular* values of the parameters that the interaction distribution is invariant, as seen below.

[6]It is important to notice that choosing $h^{+} = +\infty$ ($h^{-} = +\infty$) implies $\psi\left(0^{+}\right) = 0$ [$\psi\left(0^{-}\right) = 0$]. The choice $h^{\pm} \in \mathbb{R} \cup \{-\infty\}$ (instead of $h^{\pm} \in \mathbb{R} \cup \{+\infty\}$) in these expressions does not change the b.c., resulting in *the same* interaction. Thus, it is enough to consider the parametrization above for $h^{\pm}$, a choice of sign that will prove to be convenient in section 4.

For a *regular* potential $V(x)$, under a parity transformation, $\mathcal{P}: x \to -x$, $\psi(x) \to \psi(-x) \equiv \chi(x)$ and $V(x) \to \tilde{V}(x) \equiv V(-x)$, the Schrödinger equation changes as Schiff [39]

$$-\psi''(x) + V(x)\psi(x) = E\psi(x) \quad \xrightarrow{\mathcal{P}} \quad -\chi''(x) + \tilde{V}(x)\chi(x) = E\chi(x). \tag{26}$$

Invariance under parity is automatically fulfilled if $V(x)$ is an even function and, thus, the transformed equation is identical to the original one. Similarly, for a *regular* potential, the corresponding transformation properties of the interaction distribution follow directly from the fact that, in this case, $S[\psi, V](x) = V(x)\psi(x)$, which transforms as $S[\psi, V](x) \xrightarrow{\mathcal{P}} S[\psi, V](-x) \equiv \tilde{S}[\chi, \tilde{V}](x)$. Then, the interaction distribution is invariant (i.e., *even*) under parity if $\tilde{S}[\chi, \tilde{V}](x) = S[\chi, V](x)$, and, equivalently, the interaction distribution is *odd* under parity if $\tilde{S}[\chi, \tilde{V}](x) = -S[\chi, V](x)$.

For a singular interaction, as it is the case of the Coulomb potential considered here, as we have seen, the product $V(x)\psi(x)$ is in general ill-defined and we *must* generalize the *singular* interaction distribution using the method employed in the last section. Then, the characterization of the properties of $S[\psi, V](x)$ under a symmetry transformation is made by *extending* the behavior of this distribution in the regular case to the singular one [30]. Therefore, under a transformation of parity the distributional Schrödinger equation transforms as

$$\psi''(x) + E\,\psi(x) = S[\psi, V](x) \quad \xrightarrow{\mathcal{P}} \quad \chi''(x) + E\,\chi(x) = \tilde{S}[\chi, \tilde{V}](x),$$

and the interaction distribution is characterized as

$$- \textit{ Even}: \quad \text{if} \quad S[\psi, V](x) \quad \xrightarrow{\mathcal{P}} \quad \tilde{S}[\chi, \tilde{V}](x) = S[\chi, V](x), \tag{27}$$

$$- \textit{ Odd}: \quad \text{if} \quad S[\psi, V](x) \quad \xrightarrow{\mathcal{P}} \quad \tilde{S}[\chi, \tilde{V}](x) = -S[\chi, V](x), \tag{28}$$

regardless of whether the interaction is singular or regular. As expected, invariance under parity transformations requires an even $S[\psi, V](x)$.

Now we can consider the properties of the interaction distribution (9), with $c_0[\psi, V]$ and $c_1[\psi, V]$ given by (16) or (23), under a parity transformation. This can be further simplified by considering the behavior of $S_0[\psi, V](x)$ and the contact interactions in separate. To see how $S_0[\psi, V](x)$ behaves under parity, notice that, since $G[\psi, V](x)$ is a regular distribution, it can be represented by the ordinary function on the r.h.s. of (7). Thus, in the sense of ordinary functions, it follows that

$$\begin{aligned} G[\psi, V](-x) = \gamma \Big\{ & -\chi(x)\mathrm{sgn}(x)\ln|x| + \chi'(x)\,|x|\left(\ln|x| - 1\right) \\ & + \int_0^x \chi(t)\left(|t|E - \gamma\right)\left(\ln|t| - 1\right) dt \Big\} \\ = & -G[\chi, V](x), \end{aligned}$$

that is, the *regular* distribution $G[\psi, V](x)$ is *odd* under parity. As a consequence, since $S_0[\psi, V](x) = G'[\psi, V](x)$ (derivative in the distributional sense), we conclude that the distribution $S_0[\psi, V](x)$ is *even* under parity: $S_0[\psi, V](x) \xrightarrow{\mathcal{P}} S_0[\chi, V]$[7]. Therefore, the whole interaction term $S[\psi, V](x) = S_0[\psi, V](x) + c_0[\psi, V]\,\delta(x) + c_1[\psi, V]\,\delta'(x)$ will be *even* if, and only if, the distribution corresponding to the contact terms, $c_0[\psi, V]\,\delta(x) + c_1[\psi, V]\,\delta'(x)$ is also even, i.e., if, and only if[8]

$$c_0[\psi, V]\,\delta(-x) + c_1[\psi, V]\,\delta'(-x) = c_0[\chi, V]\,\delta(x) + c_1[\chi, V]\,\delta'(x). \tag{29}$$

In reference [30] it was shown that this condition is satisfied for permeable interactions if, and only if, the parameters in (16) satisfy

$$a = d \quad \text{and} \quad \varphi = 0, \tag{30}$$

thus reducing the allowed permeable interactions to a subfamily with only two independent parameters. For impermeable interactions, condition (29) is satisfied if, and only if, the parameters in (23) are given by

$$h^+ = -h^- = h, \quad \text{with } h \text{ finite}, \quad \text{or} \quad h^+ = h^- = +\infty, \tag{31}$$

thus reducing the allowed impermeable interactions from two parameters to just *one*. Below we present a systematic study of the properties of the bound states for the subfamily of parity invariant (even) Coulomb interactions.

4. BOUND STATES FOR PARITY INVARIANT COULOMB INTERACTIONS

For bound states ($E < 0$), the general solution for the one-dimensional Schrödinger equation with a Coulomb potential outside the origin [i.e., Equation (6)] is given by (A5), in the **Appendix 2**, and reproduced below

$$\psi(x) = \mathcal{W}_{\frac{-\gamma}{\sqrt{-4E}},\frac{1}{2}}\left(\sqrt{-4E}\,|x|\right)\left[B_-\,\theta(-x) + B_+\,\theta(x)\right]. \tag{32}$$

The relationship between the constants B_+ and B_- in this expression is established by the boundary conditions at the origin, which, in turn, are determined by the parameters of the interaction, according to the results of the sections 2.2 and 3. Let us now investigate the properties of the bound states of parity invariant Coulomb interactions in both the permeable and impermeable cases.

4.1. Permeable Interactions

For the subfamily of even interactions with a permeable origin, the boundary conditions are given by (19), with $a = d$ and $\varphi = 0$. By using the lateral limits given in the **Appendix 2** by the expressions (A6) and (A8), these boundary conditions can be written as the following system of equations for the unknown coefficients B_+ and B_-:

$$\begin{cases} W_0(E)\,B_+ + \left[b\,F_0(E) - a\,W_0(E)\right]\,B_- = 0\,; \\ \\ F_0(E)\,B_+ + \left[a\,F_0(E) - c\,W_0(E)\right]\,B_- = 0, \end{cases} \tag{33}$$

[7] It is a simple task to show that, if $f(x)$ is an *odd distribution*, then $\langle f'(x), \varphi(x)\rangle = \langle f'(-x), \varphi(x)\rangle$ [32] and, therefore, $f'(-x) = f'(x)$, i.e., the distributional derivative $f'(x)$ is an *even distribution*. Similarly, if $f(x)$ is an even distribution, its distributional derivative is odd. Hence, as with ordinary functions, taking the distributional derivative changes the parity of the (resulting) distribution.

[8] Note that $\psi(0^\pm) = \chi(0^\mp)$, $\psi'(0^\pm) = -\chi'(0^\mp)$, $\delta(-x) = \delta(x)$ and $\delta'(-x) = -\delta'(x)$.

where the functions $W_0(E)$ and $F_0(E)$ are defined in the **Appendix 2**. These equations allow for non-trivial solutions for $B_\pm$ if, and only if,

$$b\,F_0(E)^2 + c\,W_0(E)^2 - 2a\,W_0(E)\,F_0(E) = 0. \tag{34}$$

The values of E which solve this equation determine the allowed bound states energies. Below we consider separately the cases with $b \neq 0$ or $b = 0$.

4.1.1. $b \neq 0$

When $b \neq 0$, the allowed energies must be such that $W_0(E) \neq 0$. Otherwise, Equation (34) has no solution, since $F_0(E)$ and $W_0(E)$ cannot vanish simultaneously [see Equations (A10) and (A11) in the **Appendix 2**]. Therefore, Equation (34) can be rewritten in the form of a quadratic equation for $Q(E) = \frac{F_0(E)}{W_0(E)}$,

$$b\,Q(E)^2 - 2a\,Q(E) + c = 0, \tag{35}$$

whose solutions (obtained using the fact that $a^2 - bc = 1$)

$$Q^{(\pm)}(E) = \frac{a \pm 1}{b}, \tag{36}$$

are transcendental equations that determine the allowed binding energies – the explicit form and some of the properties of $Q(E)$ are given in the **Appendix 2**.

The relationship between the coefficients $B_\pm$ is obtained by substituting (35) into (33), obtaining

$$B_+^{(\pm)} = \mp B_-^{(\pm)}. \tag{37}$$

Therefore, for each value of E that solves the condition $Q^{(+)}(E)$ in (36) there is an associated eigenfunction given by (32) with $B_+^{(+)} = -B_-^{(+)}$, which is an *odd* function under parity. Similarly, for each energy E satisfying $Q^{(-)}(E)$ in (36), there is an eigenfunction (32) with $B_+^{(-)} = B_-^{(-)}$, which is an *even* function under parity. Thus, in this case, the bound states have eigenfunctions with defined parity, and their binding energies are *not* degenerate.

It is instructive to consider a plot of the function $Q(E)$ to illustrate the structure of the binding energies and the parity of the associated bound states (even though to determine the actual binding energies one needs consider a specific choice of the parameters). In **Figure 1** the two horizontal lines illustrate the two values in the r.h.s of (36), and the intersections between these lines and the graph of $Q(E)$ determine the allowed binding energies. Since $Q(E)$ is monotonic in the intervals between two successive discontinuities, as $|E|$ increases from zero the intersections will alternate between the lines—that is, the binding energies alternate between the solutions of $Q^{(+)}(E)$ and $Q^{(-)}(E)$ in (36). If $b > 0$ ($b < 0$), the intersections with the upper line correspond to the solutions of $Q^{(+)}(E)$ [$Q^{(-)}(E)$] in (36) and, therefore, to *odd* (*even*) eigenstates, whereas the energies associated to the intersections with the lower line are given by the solutions of $Q^{(-)}(E)$ [$Q^{(+)}(E)$] and, thus, correspond to *even* (*odd*) eigenstates. Therefore, as $|E|$ increases from zero we encounter *a discrete set of bound states, each one having definite parity, with the parity alternating between successive states.*

Finally, for any physically acceptable (finite) choice of the interaction parameters a, b, c ($b \neq 0$, $a^2 - bc = 1$), the r.h.s of (36) is finite. Hence, there will always be a finite largest value of $|E|$ ($E < 0$) for which the graph of $Q(E)$ intercepts the lower horizontal line, since $Q(E) \to -\infty$ as $E \to -\infty$ [see (A13) in the **Appendix 2**], corresponding to *a ground state with finite binding energy* and whose (definite) parity depends on the sign of b, as mentioned above.

4.1.2. $b = 0$

Taking $b = 0$ in (19) implies that c is arbitrary and $a = \pm 1$ (with each choice of sign corresponding to a different interaction). In this case, Equation (34) is equivalent to

$$W_0(E) = 0 \qquad \text{or} \qquad c\,W_0(E) - 2a\,F_0(E) = 0 \tag{38}$$

The first condition in (38), $W_0(E) = 0$, gives [see Equation (A10) in the **Appendix 2**]

$$E = \epsilon_n = -\frac{\gamma^2}{4n^2}, \qquad n = 1, 2, 3, \cdots \tag{39}$$

Substituting $W_0(E) = 0$ into the second equation in (33), and taking into account the fact that $F_0(\epsilon_n) \neq 0$ [see Equation (A11)], we conclude that

$$B_+ = -a\,B_-,$$

and the corresponding eigenfunctions are *odd* (*even*) under parity transformations if $a = +1$ ($a = -1$).

The second solution in (38), since $W_0(E)$ and $F_0(E)$ cannot be simultaneously zero, can be rewritten in terms of $Q(E)$ as

$$Q(E) = \frac{c}{2a}. \tag{40}$$

Substituting this condition into the first equation in (33) we obtain

$$B_+ = a\,B_-,$$

and the corresponding eigenfunctions are *even* (*odd*) if $a = +1$ ($a = -1$), thus with parity opposite to the eigenfunctions associated with the condition $W_0(E) = 0$

The values of energy that solve (40) correspond to the intersections of the curve $Q(E)$ with the horizontal line crossing the vertical axis at $\frac{c}{2a}$ (similarly to the case $b \neq 0$ that was illustrated in **Figure 1**). In the intervals between any two successive discontinuities of $Q(E)$, which occur at the energies ϵ_n, there is always exactly one such intersection, since $Q(E)$ is monotonic in these intervals. Therefore, as $|E|$ increases from zero, the allowed energies alternate between those in the set $\{\epsilon_n\}$ and the solutions of (40), with the parity of corresponding eigenstates alternating between even and odd.

In what concerns the ground state energy and the parity of the associated eigenstate, notice that while the set of energies $\{\epsilon_n\}$ is bounded from below (with the minimum energy corresponding to $n = 1$), the set of energies given by (40) is also bounded from

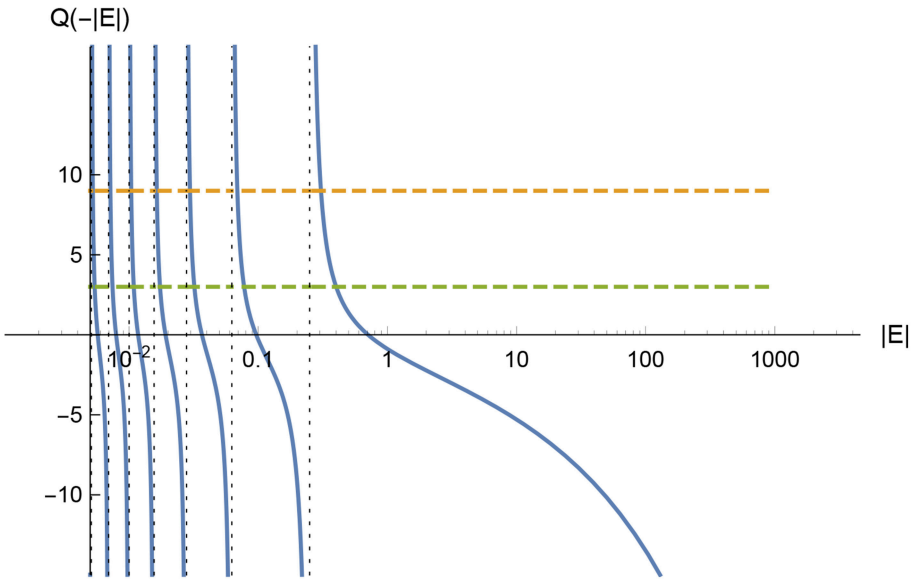

FIGURE 1 | Plot of $Q(E)$, for $E < 0$, and $\gamma = -1$ (in Rydberg atomic units). The vertical dotted lines correspond to the energies $\epsilon_n = -\frac{\gamma^2}{4n^2}$, $n = 1, 2, 3, \cdots$, for which $Q(E)$ is discontinuous [such that $W_0(\epsilon_n) = 0$]. The two horizontal lines illustrate the two values on the r.h.s of the Equation (36). If $b > 0$ ($b < 0$) the upper (lower) horizontal line correspond to $Q^{(+)}(E)$ [and $[Q^{(-)}(E)]$ in Equation (36) and to the respective b.c. in Equation (37). Since $Q(E)$ is monotonic between two discontinuity points, as the $|E|$ increases the intersections of $Q(E)$ with the horizontal lines alternate between the two lines.

below, since $c/2a$ is finite and $Q(E) \to -\infty$ when $E \to -\infty$ (see **Appendix 2**). Therefore, the ground state energy is *finite* and given by the most negative energy satisfying the condition (40), and its parity is *even* (*odd*) if $a = +1$ ($a = -1$)[9].

Having considered all the possibilities of bound states for a parity invariant Coulomb interaction with permeable origin, it is instructive to consider a few examples that illustrate these results, before proceeding to the analysis of impermeable interactions.

4.1.3. Examples of Permeable Interactions

Example 1. First, let us consider the case $a = +1, b = 0$ and c arbitrary, which corresponds to a "pure delta" interaction for the contact term in (16). In this case, the conditions for the allowed binding energies and the parity of the corresponding eigenstates are as follows.

- $W_0(E) = 0$, with binding energies given by (39) and eigenstates that are *odd* under a parity transformation.
- $Q(E) = \frac{c}{2}$, with the eigenstates having *even* parity and the binding energies given by the set of values of E such that $Q(E)$ intersects the line $c/2$ – the ground state corresponds to the most negative (finite) energy in this set.

Example 2. Consider the so-called "delta prime" interaction for the contact term in (16), i.e., $a = +1$, $b \neq 0$ and $c = 0$. In this case the allowed binding energies are given by the solutions of

- $Q^{(+)}(E) = \frac{2}{b}$, corresponding to eigenstates that are *odd* under parity. If $b < 0$, the ground state will correspond to the lowest (finite) energy of this set.
- $Q^{(-)}(E) = 0$, resulting in *even* eigenstates. If $b > 0$, the eigenstate is given by the lowest (finite) energy in this set.

Example 3. As our third example, we consider the "pure Coulomb" interaction, identified by the *absence of a contact term* in (16), i.e., $S[\psi, V] = S_0[\psi, V]$[10] [7] – obtained by choosing the parameters $a = 1$, $b = c = 0$. In this case the binding energies satisfy:

- $W_0(E) = 0$, which results in *odd* eigenstates with eigenvalues given by (39).
- $Q(E) = 0$, with the allowed energies corresponding to the intersection points of $Q(E)$ with the horizontal axis (see **Figure 1**), and eigenstates that are *even* under parity. The ground state is the lowest (finite) energy in this set.

4.2. Impermeable Interactions

At the end of the section 3 we saw that an impermeable interaction is *even* under parity if the parameters $h^{\pm}$ in (22) are such that $h^+ = -h^- = h$ (for h real and finite), or $h^+ = h^- = +\infty$. Below we consider these two cases separately.

4.2.1. h Real and Finite

For impermeable interactions satisfying $h^+ = -h^- = h$ with h finite, using (A6) and (A8), the boundary conditions (22) imply

$$\left[F_0(E) - h\, W_0(E)\right] B_{\pm} = 0, \tag{41}$$

[9]That the ground state energy E_g will always belong to the set of energies satisfying (40) can be seen from the fact that, as $|E|$ increases, the last intersection between $Q(E)$ and the horizontal line $\frac{c}{2a}$ will always occur at an energy $E_g < \epsilon_1$.

[10]This interaction is sometimes identified by the so-called "periodic" boundary conditions $\psi(0^+) = \psi(0^-)$ and $\tilde{\phi}(0^+) = \tilde{\phi}(0^-)$

which has non-trivial solutions for $B_\pm$ if, and only if,

$$F_0(E) = h\, W_0(E). \tag{42}$$

This condition is never satisfied if $W_0(E) = 0$, since $F_0(E) = 0$ and $W_0(E)$ do not vanish simultaneously (see **Appendix 2**). Therefore, (42) can be satisfied only if $W_0 \neq 0$, in which case it can be rewritten as a condition for $Q(E)$,

$$Q(E) = h. \tag{43}$$

For each energy satisfying this condition, the system (41) allows arbitrary solutions for B_+ and B_- and, as expected, these coefficients are not connected through the origin due to the impermeability of the interaction. Thus, in this case, each binding energy is *doubly degenerated*. In addition, since the *interaction* is even, it is always possible to choose the pair of eigenfunctions associated with each energy eigenvalue to have definite parity (that is, one eigenfunction *even*, the other *odd*).

Once again, the set of allowed binding energies given by Equation (43) can be graphically visualized as the energies at which the graph of $Q(E)$ intersects the *single* horizontal line crossing the vertical axis at the finite height h (which can be zero, positive or negative), similarly to the situation depicted in **Figure 1**. From the finiteness of h and the fact that $Q(E) \to -\infty$ when $E \to -\infty$, it follows that the doubly degenerated ground state has *finite* energy – the ground state binding energy can be made *arbitrarily large,* by taking h sufficiently large and negative, but it is still *finite*, since in this case h is not allowed to assume infinite values. Finally, a glance at the graph of $Q(E)$ in **Figure 1** shows that for large $h > 0$ the binding energies tend to the set $\{\epsilon_n\}$, i.e., to the energies associated to the discontinuities of $Q(E)$.

4.2.2. $h = +\infty$

Let us now consider the last remaining possibility for a parity invariant (even) Coulomb interaction, namely, the impermeable case given by the choice $h^+ = h^- = h = +\infty$ in (22). As we mentioned before, this is equivalent to imposing Dirichlet b.c. [7]

$$\psi\left(0^\pm\right) = 0, \tag{44}$$

with $\tilde{\phi}\left(0^\pm\right)$ assuming arbitrary values. By using the expressions (A6) and (A8) from the **Appendix 2**, Equation (44) can be rewritten as

$$B_\pm\, W_0(E) = 0, \tag{45}$$

which results in non-trivial solutions for $B_\pm$ if, and only if, the binding energies satisfy $W_0(E) = 0$, that is, the eigenvalues of energy are given by (39). Similarly to the previous case, conditions (45) with $W_0(E) = 0$ allow arbitrary values for the coefficients $B_\pm$, resulting in *doubly degenerated* energy eigenvalues and, as before, the pair of eigenfunctions associated with each ϵ_n can be chosen to be formed by an even and an odd eigenfunction.

Finally, we observe that the results for the case being considered here can be obtained as the limit $h \to +\infty$ of the previous case, subsection 4.2.1. However, we emphasize that the present case *cannot* be obtained from the results in the previous subsection by taking the limit $h \to -\infty$, since this would imply that the ground state energy tends to $E = -\infty$, violating the requirement $W_0(E) = 0$ [notice that $\lim_{E\to-\infty} W_0(E) = 1$ as seen in (A12)].

5. CONCLUSION

We investigated the one-dimensional hydrogen atom, with an 1D Coulomb interaction given by (3), by extending the distributional method, introduced in Calçada et al. [30] for contact interactions, to treat long-range interactions exhibiting a point singularity. After showing that the non-integrable singularity of the potential at the origin renders the ordinary Schrödinger equation ill-defined, we introduced a distributional Schrödinger equation, Equation (5), with an interaction distribution $S[\psi, V]$ to be determined from the fundamental physical and mathematical requirements **R1**–**R4**, which follow from the general structure of quantum mechanics (section 2.2)—these requirements are expected to be satisfied by *any* interaction. Requirements **R1** – **R4** allowed us to define the interaction rigorously—no ill-defined

TABLE 1 | Bound state energies and properties under parity of the corresponding eigenstates, for all subfamilies of parity invariant (even) attractive Coulomb interactions.

Interaction	Bound states energies	Eigenstates	Ground state
Permeable	$Q(E) = \frac{a+1}{b}$	odd	Finite energy
$b \neq 0$	$Q(E) = \frac{a-1}{b}$	even	(even) (odd) if ($b > 0$) ($b < 0$)
Permeable	$W_0(E) = 0$	odd (even) if $a = +1$ ($a = -1$)	Finite energy
$b = 0$			
$a = \pm 1$	$Q(E) = \frac{c}{2a}$	even (odd) if $a = +1$ ($a = -1$)	even (odd) if $a = +1$ ($a = -1$)
Impermeable		Doubly degenerated	Finite energy
	$Q(E) = h$		Doubly degenerated
h real and finite		(even and odd eigenstates)	(even and odd eigenstates)
Impermeable		Doubly degenerated	Finite energy
(Dirichlet)	$W_0(E) = 0$		Doubly degenerated
$h = +\infty$		(even and odd eigenstates)	(even and odd eigenstates)

The binding energies associated to the zeros of $W_0(E)$ are given by Equation (39). For permeable origin interactions, the parity alternates between successive bound states.

steps or infinities ever appear—and to restrict the interaction to a long range term outside the origin plus a family of contact interactions at the origin. The contact terms are obtained up to a four-parameter family of contact interactions, for the case of a penetrable origin, or up to a two-parameter family of interactions in the case of an impenetrable origin, in complete agreement with the SAE method (see, e.g., [7] and references therein).

The requirements **R1** – **R4** are not enough to completely specify the interaction and, in particular, cannot determine the specific b.c. at the origin—additional *physical* input is necessary to that end. As it is well-known, symmetry is an excellent guide in these circumstances. Therefore, since the Coulomb *potential* is even under parity transformations, it is natural to require that the interaction distribution $S[\psi, V]$ associated with this potential also be invariant (even) under parity. We stress that the invariance of the Coulomb *potential* ($V(x) = \frac{\gamma}{|x|}, x \neq 0$) under parity transformations is not sufficient to ensure that the *interaction* will be even under parity—information about the contact term is crucial to address this issue. In this context, it should be noticed that by providing an explicit form for $S[\psi, V]$, the distributional approach proves to be particularly adequate to deal with symmetry transformations. We have taken advantage of the explicit expression for the most general Coulomb *distribution* (i.e., the interaction distribution) to prove, in section 3, that the long-range term $S_0[\psi, V]$ is even under parity transformations. In this way, we concluded that the parity invariance of the total Coulomb interaction can be ensured if, and only if, the contact term also is invariant under parity transformations. As a consequence, we have shown that the *additional* requirement of parity invariance further reduces the possible contact terms associated with the generalized Coulomb interaction to a two-parameter family [26] (penetrable origin case) or a one-parameter interaction (impenetrable case). This, of course, still leaves considerable freedom in the choice of the b.c. at the origin, leading to several possible extensions of the Coulomb interaction—to further specify the interaction, additional input from the experimental situation must be considered [26, 34].

After giving a complete characterization of the subfamily of all parity invariant (attractive) Coulomb interactions, we conducted a *systematic study of the bound states* for all possible interactions in this subfamily. A summary of the results obtained is presented in **Table 1**, for convenience. From our analysis it follows that for parity invariant Coulomb interactions:

(i) the ground state energy is always *finite*;
(ii) for *permeable* interactions, the bound state energies are always *non degenerated* and the corresponding eigenfunctions have *definite parity* (which alternates between even and odd for successive bound states).
(iii) for *impermeable* interactions, *all* the bound states energies are *doubly degenerated* and, for each binding energy, the corresponding pair of eigenfunctions can be chosen to have a definite parity (with one degenerate eigenfunction even and the other odd).

Thus, our results, obtained from a mathematically well-defined treatment of the 1D Hydrogen atom, clarify the highly controversial issues concerning the boundedness of the ground state and the parity as well as the degenerescence of the bound states (see [6] and references therein).

Finally, this work demonstrates that the method developed in Calçada et al. [30] for contact interactions can be generalized for long-range interactions having point singularities (in fact, it makes essential use of the results derived in Calçada et al. [30]). The distributional approach proves to be particularly suited for symmetry analyses (see also [31]), in addition to being a physically appealing alternative to SAE methods, and it could be used to investigate other one-dimensional singular interactions such as the $1/x^2$ potential. In particular, for *odd* interactions (such as the $1/x$ potential) the approach here developed specifies completely the interaction, since there exists no 1D odd contact interaction [30]. Finally, an important open problem is the generalization of the distributional approach to higher dimensions.

DATA AVAILABILITY

All datasets generated for this study are included in the manuscript and/or the supplementary files.

AUTHOR CONTRIBUTIONS

All the authors participated in the formulation of the problem and in the calculations. JL and LM wrote the manuscript. MC, WM, and MP revised the text.

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1. APPENDIX: BASIC NOTIONS ON SCHWARTZ'S DISTRIBUTION THEORY

In this Appendix, for convenience of the reader, we briefly present some of the concepts of the Schwartz distribution theory that are directly necessary for an understanding of the main text. For an extensive presentation of distribution theory we refer to Zemanian [32].

A *distribution* f is a *continuous linear* (complex) *functional* on a *space of test functions*. Here we will consider the test functions space as the space $\mathcal{D}_0$ formed by all the (complex-valued) functions $\varphi(x)$, defined on the entire real line, which are infinitely smooth and have compact support (i.e., they vanish outside some finite interval, which does not need to be the same for all the test functions).

Let φ be a test function, and f be a distribution. The complex number associate to φ by the distribution f is denoted by $\langle f, \varphi \rangle$. If $f(x)$ is a *locally integrable* function (i.e., a function which is Lebesgue integrable over every finite interval), then the distribution f associated to the function $f(x)$ is said to be regular, and it is given by

$$\langle f, \varphi \rangle = \int_{-\infty}^{\infty} f(x)\, \varphi(x)\, dx\,,$$

for any test function φ. Distributions that can not be associated in this way to locally integrable functions are said to be *singular* — a well-known example is the Dirac delta functional δ, defined by $\langle \delta, \varphi \rangle = \varphi(0)$, $\forall\, \varphi$. When a distribution is regular we will not distinguish between the function and the regular distribution associated to it, and we will often use the abusive notation $f(x)$ to refer to the distribution f (even for singular distributions).

Any distribution can be infinitely differentiated. Denoting the n-th derivative of a test function or a distribution by a superscript (n), we have

$$\left\langle f^{(n)}, \varphi \right\rangle \equiv (-1)^n \left\langle f, \varphi^{(n)} \right\rangle,$$

for all test functions φ. Every distribution has primitives (indefinite integrals), and any two primitives of a given distribution differ by a constant. We denote the primitive of a distribution or test function by the superscript (-1). Considering a fixed test function φ_0 satisfying $\int_{-\infty}^{\infty} \varphi_0(x)\ dx = 1$, a *primitive* of f is a distribution $f^{(-1)}$ defined as

$$\left\langle f^{(-1)}, \varphi \right\rangle \equiv \langle c, \varphi \rangle - \langle f, \psi \rangle, \quad \forall\, \varphi$$

where c is an arbitrary constant, $\psi(x) = \int_{-\infty}^{x} \chi(t)\ dt$ and $\chi(x) = \varphi(x) - \varphi_0(x) \int_{-\infty}^{\infty} \varphi(t)\ dt$.

On any closed finite interval I every distribution f can be written as the $(r+2)$-th order derivative of a distribution h associated to a continuous function whose derivative is not continuous in this interval (in the ordinary sense) — see [32], p. 162. In other words, $\langle f, \varphi \rangle = \left\langle h^{(r+2)}, \varphi \right\rangle$, for all φ with support in I. The integer r is the *order* of the distribution f. Therefore, if $r = -2$ the distribution f corresponds to a continuous function whose derivative is not continuous on the interval I; if $r = -1$, f is the derivative of a continuous distribution, but f is not continuous; if $r = 0$, f is not locally integrable and corresponds to a *singular* distributon (since $f^{(-1)}$ is not continuous). Summarizing, $r \leq -2$ characterizes distributions that correspond to continuous functions (regular distributions), $r \geq 0$ characterizes singular distributions, and distributions with $r = -1$ may be either singular or regular. If $r = -\infty$ the distribution is infinitely smooth on I (see [32], p. 162, for details). When the order is finite, differentiation increases the order by one, whereas indefinite integration decreases the order by one. The order of a finite sum of distributions is the maximum order among the various terms, except when the distributions of largest order cancel each other, resulting a lower order for the sum [32].

Two distributions f and g are said to be *equal* on an open set I if they associate the same number $\langle f, \varphi \rangle = \langle g, \varphi \rangle$ to every test function φ whose support is contained in I (if $I = \mathbb{R}$ then the two distributions are simply said to be equal). Two functions that are locally integrable and differ on a set of zero Lebesgue measure define the *same* distribution. Thus, the same regular distribution is associated to the class of all locally integrable functions which differ among themselves only on a set of zero Lebesgue measure.

Any distribution f can be multiplied by an *infinitely smooth function* $\eta(x)$, resulting in a new distribution ηf, according to $\langle \eta f, \varphi \rangle \equiv \langle f, \eta \varphi \rangle$. If f and g are two locally integrable functions such that their product fg is also locally integrable, then the product of the corresponding regular distributions exists, and it is the regular distribution defined as

$$\langle f\, g, \varphi \rangle \equiv \int_{-\infty}^{\infty} f(x) g(x)\, \varphi(x)\, dx, \qquad \forall\, \varphi.$$

However, it is an important fact of Schwartz's distribution theory that the product of two *arbitrary* distributions cannot be defined in a unique way. For example, the function $f(x) = \frac{1}{\sqrt{|x|}}$ is locally integrable and thus defines a regular distribution. The function $g(x) = \frac{1}{|x|}$, on the other hand, *is not integrable on any interval including the origin*. Therefore, the product $f^2(x) = g(x)$ does not define a regular distribution (in addition, one can define *several non-equivalent singular* distributions which coincide with $\frac{1}{|x|}$ over any interval *which does not include the origin*).

The following Theorem and its corollary are of crucial importance in this work.

Theorem. Zemanian ([32], p. 98) A necessary and sufficient condition for a distribution $f(x)$ on $\mathbb{R}$ to have a support consisting of a single point x_0 is that it be a finite sum

$$f(x) = \sum_{n=0}^{r_m} a_n \delta^{(n)}\,(x - x_0)\,, \tag{A1}$$

where the a_n are constants, $a_{r_m} \neq 0$, and r_m is the singular order of the distribution f.

As a corollary, it follows that if two distributions f and g are equal on the open region $\mathbb{R}\backslash\{0\}$, then their difference $f-g$ must have its support concentrated at a single point (the origin), and it is a finite linear combination of the delta distribution and its derivatives.

2. APPENDIX: BOUND STATES OF THE 1-D HYDROGEN ATOM

Here we present some properties of the (well-known) bound state solutions of the Schrödinger equation for the 1D Hydrogen atom, given by (6), on the disjoint union $(-\infty,0)\cup(0,+\infty)$. By performing the change of variable $z=\sqrt{-4E}\,|x|$, $x\neq 0$, Equation (6) becomes a special case of the Whittaker equation, namely [40]

$$\beta''(z)+\left(\frac{\tilde{\gamma}}{z}-\frac{1}{4}\right)\beta(z)=0,\quad z\neq 0, \tag{A2}$$

with $\tilde{\gamma}=\frac{-\gamma}{\sqrt{-4E}}$. For bound states ($E<0$), both z and $\tilde{\gamma}$ are real and positive (since in this work we are considering only the attractive Coulomb potential, $\gamma<0$). The two linearly independent solutions of Whittaker's equation, Equation (A2), are [40]

$$\mathcal{M}_{\tilde{\gamma},\frac{1}{2}}(z)=z\,\mathrm{e}^{-\frac{z}{2}}\,M\left(1-\tilde{\gamma},2,z\right), \tag{A3}$$

$$\mathcal{W}_{\tilde{\gamma},\frac{1}{2}}(z)=z\,\mathrm{e}^{-\frac{z}{2}}\,U\left(1-\tilde{\gamma},2,z\right) \tag{A4}$$

where $M\left(a,b,z\right)$ and $U(a,b,z)$ are the confluent hypergeometric functions of the first and of the second kind, respectively.

For negative energies $\mathcal{M}_{\frac{-\gamma}{\sqrt{-4E}},\frac{1}{2}}\left(\sqrt{-4E}|x|\right)$ is not an acceptable solution, since it diverges when $|x|\to\infty$. Therefore, the general solution of (A2) for bound states is

$$\psi(x)=\mathcal{W}_{\frac{-\gamma}{\sqrt{-4E}},\frac{1}{2}}\left(\sqrt{-4E}\,|x|\right)\left[B_-\,\theta(-x)+B_+\,\theta(x)\right], \tag{A5}$$

where $\theta(x)$ is the Heaviside theta function and the arbitrary constants $B_\pm$ must be related by the boundary conditions at the origin, which depend on the specific choice of the parameters determining the interaction (see section 2.2). It follows from the properties of the Whittaker functions (see [40], Ch. 13) that $\psi(x)$ has finite limits at both sides of the origin, namely

$$\psi\left(0^\pm\right)=B_\pm\,\mathcal{W}_{\frac{-\gamma}{\sqrt{-4E}},\frac{1}{2}}\,(0)=B_\pm\,W_0\,(E)\,, \tag{A6}$$

where we have defined

$$W_0\,(E)\equiv\frac{1}{\Gamma\left(1+\frac{\gamma}{\sqrt{-4E}}\right)}\,. \tag{A7}$$

In section 2 the function $\tilde{\phi}(x)$, Equation (12), was introduced and shown to have finite lateral limits at both sides of the origin. From (A5), these lateral limits can be explicitly obtained as

$$\tilde{\phi}\left(0^\pm\right)=\pm B_\pm\,F_0\,(E)\,, \tag{A8}$$

with

$$\begin{aligned}&F_0\,(E)=W_0(E)\,Q(E),\\&Q(E)=\left[\frac{1}{2}\gamma\log(-4E)+\gamma\,\psi^{(0)}\left(\frac{\gamma}{2\sqrt{-E}}\right)+2\gamma'\gamma+\sqrt{-E}\right],\end{aligned} \tag{A9}$$

where γ' is the Euler's constant and $\psi^{(0)}(x)$ is the digamma function, defined as $\psi^{(0)}(x)=\frac{1}{\Gamma(x)}\frac{d}{dx}\Gamma(x)$ [40].

The functions $W_0(E)$, $F_0(E)$ and $Q(E)$ have the following important properties, which are used in the main text of the paper.

- $W_0(E)$ is continuous and has simple zeros at the points in which the gamma function in (A7) diverges, namely at

$$E=\epsilon_n=-\frac{\gamma^2}{4n^2},\quad n=1,2,3,\cdots. \tag{A10}$$

- $F_0\,(E)$ is continuous, and at the zeros of $W_0(E)$ it assumes the nonzero values

$$F_0(\epsilon_n)=(-1)^n(n-1)!\,\gamma,\quad n=1,2,3,\cdots. \tag{A11}$$

- $Q(E)=\frac{F_0(E)}{W_0(E)}$ is continuous in any interval $E\in(\epsilon_n,\epsilon_{n+1})$, with n a positive integer. At the boundaries of these intervals $Q(E)$ diverges.
- In the limit $E\to-\infty$ we have

$$\lim_{E\to-\infty}W_0(E)=1, \tag{A12}$$

$$\lim_{E\to-\infty}Q(E)=-\infty, \tag{A13}$$

$$\lim_{E\to-\infty}F_0(E)=-\infty. \tag{A14}$$

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The Birman-Schwinger Operator for a Parabolic Quantum Well in a Zero-Thickness Layer in the Presence of a Two-Dimensional Attractive Gaussian Impurity

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In this note we consider a quantum mechanical particle moving inside an infinitesimally thin layer constrained by a parabolic well in the x-direction and, moreover, in the presence of an impurity modeled by an attractive Gaussian potential. We investigate the Birman-Schwinger operator associated to a model assuming the presence of a Gaussian impurity inside the layer and prove that such an integral operator is Hilbert-Schmidt, which allows the use of the modified Fredholm determinant in order to compute the bound states created by the impurity. Furthermore, we consider the case where the Gaussian potential degenerates to a δ-potential in the x-direction and a Gaussian potential in the y-direction. We construct the corresponding self-adjoint Hamiltonian and prove that it is the limit in the norm resolvent sense of a sequence of corresponding Hamiltonians with suitably scaled Gaussian potentials. Satisfactory bounds on the ground state energies of all Hamiltonians involved are exhibited.

Keywords: Gaussian potential, Birman-Schwinger operator, Hilbert-Schmidt operator, contact interaction, quantum well

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1. INTRODUCTION

The study of point potentials in Quantum Physics has recently received a lot of attention for a wide range of interests. First of all, point potentials serve as solvable or quasi-solvable models that approximate the action of intense and very short range potentials [1–3]. They have been used to model several kinds of extra thin structures [4, 5], to mimic point defects in materials, or to study heterostructures [6–9]. In addition, point potentials play a role in modeling impurities in quantum field theory [10–13]. Furthermore, they play an important role after a recent interpretation of the Casimir effect [14, 15]. The unexpected relations between contact potentials and group theory should also be noted [16]. They also play a role in modeling Kronig-Penney crystals in condensed matter physics in various dimensions [1, 17–22].

More examples of physical applications of this kind of interactions are: Bose-Einstein condensation in a harmonic trap with a tight and deep "dimple" potential, modeled by a Dirac delta function [23]; non-perturbative study of the entanglement of two directed polymers subjected to

repulsive interactions given by a Dirac δ-function potential [24]; a periodic array of Dirac delta interactions is useful to investigate the light propagation in a one-dimensional realistic dielectric superlattice, which has been investigated for the transverse electric and magnetic fields and for omnidirectional polarization modes [25–27].

One-dimensional quantum models with contact interactions are also useful to study a wide range of quantum properties, including scattering, since these models are quite often solvable. They also serve to acquire experience in order to analyse systems with contact potentials in higher dimensions. However, an important difference is to be pointed out: while one-dimensional contact potentials are usually defined through matching conditions at isolated points, their proper definition in higher dimensions requires a process of regularization.

Quantum two-dimensional systems are particularly interesting for their physical applications. In this particular context, the graphene deserves a special mention because of its importance, although this is not the only one two-dimensional quantum system of interest in physics. From a theoretical point of view, quantum theory in two dimensions has not yet been developed to the same extent of its one-dimensional and three-dimensional analogs, in spite of its enormous interest. Although two-dimensional quantum systems look rather simple, due to the presence of logarithmic singularities in the resolvent kernel of their free Hamiltonian, their level of complexity and, hence, their difficulty of study is far higher than the one-dimensional case (and, to a great extent, the three-dimensional case).

An important contribution to the understanding of two-dimensional quantum mechanics was provided by Duclos' article [28] on the two-dimensional hydrogen atom perturbed by a point interaction, a model that had not been dealt with in Albeverio et al. [1]. One of the main results of that paper is that the free Hamiltonian of that model, namely that of the 2D hydrogen atom, was rigorously shown to be the norm resolvent limit of the Hamiltonian of the 3D Hamiltonian of the hydrogen atom confined to an infinite planar slab of width $a > 0$ as $a \to 0_+$.

A remarkable feature of two-dimensional models with contact interactions, manifesting itself even in the simple case of the negative Laplacian perturbed by a point interaction, is represented by their peculiar dependence of the bound state energies on the coupling constant. As is well known, the one-dimensional model exhibits a single bound state only when the point interaction is attractive and the eigenvalue is a quadratic function of the strength of the interaction. The three-dimensional case also exhibits a single bound state only in the attractive case but the eigenvalue depends quadratically on the reciprocal of the renormalized coupling constant. In two dimensions the bound state keeps existing even if the contact interaction is repulsive and the dependence becomes exponential (see [1]). The latter behavior is confirmed even when a confinement potential is present in addition to the contact potential, which physically mimics the presence of impurities or thin barriers in the material inside which the quantum particle is moving [29, 30].

In this note, partly motivated by Duclos' paper, we intend to study a different two-dimensional model with the free Hamiltonian given by:

$$H_0 = \left(-\frac{1}{2}\frac{d^2}{dx^2} + \frac{x^2}{2}\right) - \frac{1}{2}\frac{d^2}{dy^2}\,, \tag{1.1}$$

to which we add an attractive impurity assumed to be modeled by the isotropic Gaussian potential

$$W(x,y) = -\lambda V(x,y) = -\lambda e^{-(x^2+y^2)}, \quad \lambda > 0\,, \tag{1.2}$$

so that the total Hamiltonian is

$$H_\lambda = H_0 + W(x,y) = H_0 - \lambda V(x,y) = H_0 - \lambda e^{-(x^2+y^2)}, \quad \lambda > 0. \tag{1.3}$$

It is worth mentioning that the recent literature [31–34] has shown a renewed interest in the spectral analysis of the one-dimensional Hamiltonian with a Gaussian potential, namely

$$H := -\frac{1}{2}\frac{d^2}{dx^2} - \lambda\, e^{-x^2/2}, \quad \lambda > 0. \tag{1.4}$$

Therefore, (1.3) could also be regarded as a possible two-dimensional generalization of (1.4).

At this point, it is interesting to recall that a three-dimensional material with confinement in only one dimension is said to be a quantum well [35], while a 3D material with two-dimensional confinement is called a quantum wire. Therefore, in the limiting case of a quantum well inside a layer with zero thickness, it makes sense to consider the model in which the confining potential is parabolic. Due to the mathematical subtleties required, in this note we have chosen to omit the proof of the resolvent convergence of the Hamiltonian of a three-dimensional parabolic quantum well inside a thin layer to the 2D Hamiltonian (1.3) as the thickness of the layer vanishes.

Instead we start directly by writing the Green function of the two-dimensional Hamiltonian with a one-dimensional harmonic potential. Once a perturbation given by an attractive two-dimensional Gaussian potential is added, we study the properties of the corresponding Birman-Schwinger operator, that is to say the crucial part in the interaction term of the resolvent of the perturbed Hamiltonian. We remind the reader that the resolvent is the key to obtain the energy eigenvalues. We later consider the model in which the 2D Gaussian impurity potential gets replaced by one having a Dirac delta for the coordinate subjected to the harmonic confinement maintaining the Gaussian character for the other coordinate.

It may be worth pointing out that the Hamiltonian (1.1) has been used by Dell'Antonio and collaborators [36] as the free Hamiltonian in the model of a quantum system consisting of two one-dimensional particles, one of which is harmonically bound to its equilibrium position, mutually interacting by means of the contact interaction $\delta(x-y)$. In other words, the interaction studied in [36] will be replaced by the one in (1.2).

Solving the eigenvalue problem for this kind of Hamiltonians is not, in general, an easy task and often requires rather sophisticated tools. One of the most widely used is the Birman-Schwinger operator, namely the integral operator

$$B_E = (\operatorname{sgn} W)|W|^{\frac{1}{2}}(H_0 - E)^{-1}|W|^{\frac{1}{2}}, \tag{1.5}$$

and the related technique: as in most applications B_E can be shown to be compact, the solutions of the eigenvalue problem for the Hamiltonian are given by those values of E for which B_E has an eigenvalue equal to -1 (see [22, 37, 38] and references therein as well as [39], p. 99). Therefore, the detailed study of the properties of the Birman-Schwinger operator arising from our model is quite relevant. In the present note, we show that the Birman-Schwinger operator is Hilbert-Schmidt. We also show that H_λ is self-adjoint and bounded from below.

In addition, H_λ has a special relation with a kind of two-dimensional contact operator that will be studied in section 2.1. This is given by the Hamiltonian described heuristically by

$$H_\lambda^\delta = H_0 - \lambda\sqrt{\pi}\,\delta(x)\,e^{-y^2}, \lambda > 0, \tag{1.6}$$

where $\delta(x)$ is the Dirac delta centered at the origin. We show that H_λ^δ is self-adjoint on a natural domain and can be obtained as the limit in the norm resolvent sense as $n \longmapsto \infty$ of the following sequence of Hamiltonians:

$$H_{n,\lambda} := H_0 - \lambda n\, e^{-(n^2x^2+y^2)}, \lambda > 0, \tag{1.7}$$

thus with Gaussian type potentials (as was the case for H_λ) which become increasingly more attractive and anisotropic as n goes to infinity.

Finally, it will be shown that the Hamiltonian H_λ (resp. H_λ^δ) is bounded from below and its lower bound can be obtained using a certain transcendental equation.

2. THE BIRMAN-SCHWINGER OPERATOR FOR OUR MODEL

Starting from the Hamiltonian H_0 in (1.1), it is rather straightforward to infer that the associated Green function, namely the integral kernel of the resolvent operator, reads for any $E < \frac{1}{2}$:

$$(H_0 - E)^{-1}(x,x',y,y') = \sum_{n=0}^{\infty} \frac{e^{-\sqrt{2\left(n+\frac{1}{2}-E\right)}\,|y-y'|}}{\sqrt{2\left(n+\frac{1}{2}-E\right)}}\,\phi_n(x)\phi_n(x'), \tag{2.1}$$

where $\phi_n(x)$ is the normalized n-th eigenfunction of the one-dimensional harmonic oscillator.

Once the above attractive Gaussian perturbation (1.2) is added, the total Hamiltonian is H_λ in (1.3). Therefore, its associated Birman-Schwinger integral kernel [22, 31, 32, 37, 38, 40, 41] given by (1.5) is:

$$\begin{aligned} B_E &= -\lambda\,\tilde{B}_E\left(x,x_1,y,y_1\right) = -\lambda\,|V|^{\frac{1}{2}}\,(H_0-E)^{-1}\,|V|^{\frac{1}{2}}\,(x,x_1,y,y_1) = \\ &= -\lambda e^{-(x^2+y^2)/2}\left[\sum_{n=0}^{\infty}\frac{e^{-\sqrt{2\left(n+\frac{1}{2}-E\right)}|y-y_1|}}{\sqrt{2\left(n+\frac{1}{2}-E\right)}}\phi_n(x)\phi_n(x_1)\right]e^{-(x_1^2+y_1^2)/2}, \end{aligned} \tag{2.2}$$

The main goal of this brief note is to rigorously prove that such an integral operator is Hilbert-Schmidt, that is to say $\mathrm{tr}(\tilde{B}_E^2) < \infty$, given the evident positivity of the operator $\tilde{B}_E$ (and our choice $\lambda > 0$). As the kernel of the positive operator $\tilde{B}_E^2$ is clearly

$$\begin{aligned} \tilde{B}_E^2\left(x,x_2,y,y_2\right) &= e^{-(x^2+y^2)/2}\left\{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left[\sum_{m=0}^{\infty}\frac{e^{-\sqrt{2\left(m+\frac{1}{2}-E\right)}|y-y'|}}{\sqrt{2\left(m+\frac{1}{2}-E\right)}}\phi_m(x)\phi_m(x')\right]\right. \\ &\left.\times\, e^{-(x'^2+y'^2)}\left[\sum_{n=0}^{\infty}\frac{e^{-\sqrt{2\left(n+\frac{1}{2}-E\right)}|y'-y_2|}}{\sqrt{2\left(n+\frac{1}{2}-E\right)}}\phi_n(x')\phi_n(x_2)\right]dx'dy'\right\}e^{-(x_2^2+y_2^2)/2}, \end{aligned} \tag{2.3}$$

its trace reads

$$\begin{aligned} \mathrm{tr}(\tilde{B}_E^2) &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\tilde{B}_E^2\left(x,x,y,y\right)dxdy \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}dxdydx'dy'\,e^{-(x^2+y^2)}e^{-(x'^2+y'^2)} \\ &\quad\times\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{e^{-\left(\sqrt{2\left(m+\frac{1}{2}-E\right)}+\sqrt{2\left(n+\frac{1}{2}-E\right)}\right)|y-y'|}}{2\sqrt{\left(m+\frac{1}{2}-E\right)\left(n+\frac{1}{2}-E\right)}} \\ &\quad\phi_m(x)\phi_m(x')\phi_n(x)\phi_n(x'). \end{aligned} \tag{2.4}$$

The latter multiple integral can be rewritten as:

$$\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\left[\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{-y^2}\frac{e^{-\left(\sqrt{2\left(m+\frac{1}{2}-E\right)}+\sqrt{2\left(n+\frac{1}{2}-E\right)}\right)|y-y'|}}{2\sqrt{\left(m+\frac{1}{2}-E\right)\left(n+\frac{1}{2}-E\right)}}e^{-y'^2}dydy'\right] \left\langle\phi_m, e^{-(\cdot)^2}\phi_n\right\rangle^2 \tag{2.5}$$

where $\langle f,g\rangle$ denotes the standard scalar product of the two functions.

Let us consider the double integral in (2.5). With the notation,

$$f(y-y') := e^{-\left(\sqrt{2\left(m+\frac{1}{2}-E\right)}+\sqrt{2\left(n+\frac{1}{2}-E\right)}\right)|y-y'|}, \qquad g(y') = e^{-y'^2}, \tag{2.6}$$

the second integral becomes the convolution $(f*g)(y)$, so that the double integral may be written as

$$\frac{1}{2\sqrt{\left(m+\frac{1}{2}-E\right)\left(n+\frac{1}{2}-E\right)}}\int_{-\infty}^{\infty}e^{-y^2}\left[(f*g)(y)\right]dy\,. \tag{2.7}$$

Using the Schwarz inequality (2.7) is smaller than or equal to

$$\frac{1}{2\sqrt{(m+\frac{1}{2}-E)(n+\frac{1}{2}-E)}}||e^{-(\cdot)^2}||_2\,||f*g||_2\,, \tag{2.8}$$

where $||\cdot||_p$ denotes the norm in $L^p(\mathbb{R})$. Young's inequality [42] shows that

$$||f*g||_r \leq ||f||_p\,||g||_q\,, \qquad \text{with} \qquad \frac{1}{p}+\frac{1}{q}=\frac{1}{r}+1\,. \tag{2.9}$$

Therefore, with $p=r=2$ and $q=1$, it follows that (2.8) is smaller than or equal to

$$\frac{1}{2\sqrt{(m+\frac{1}{2}-E)(n+\frac{1}{2}-E)}}\,||e^{-(\cdot)^2}||_2^2\,||f||_1\,. \tag{2.10}$$

The two norms in (2.9) yield two integrals which can be easily computed, so as to obtain

$$\frac{\sqrt{\pi}}{2^{\frac{3}{2}}\sqrt{(m+\frac{1}{2}-E)(n+\frac{1}{2}-E)}\left(\sqrt{2(m+\frac{1}{2}-E)}+\sqrt{2(n+\frac{1}{2}-E)}\right)}$$

$$\leq \frac{\sqrt{\pi}}{4(m+\frac{1}{2}-E)^{\frac{3}{4}}(n+\frac{1}{2}-E)^{\frac{3}{4}}}\,. \tag{2.11}$$

Hence, the trace (2.4) is bounded by:

$$\begin{aligned}\mathrm{tr}(\tilde{B}_E^2) \;&\leq\; \frac{\sqrt{\pi}}{4}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{\left\langle\phi_m, e^{-(\cdot)^2}\phi_n\right\rangle^2}{(m+\frac{1}{2}-E)^{\frac{3}{4}}(n+\frac{1}{2}-E)^{\frac{3}{4}}}\\ &=\; \frac{\pi^{\frac{3}{2}}}{4}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{\langle\phi_m\phi_0,\phi_0\phi_n\rangle^2}{(m+\frac{1}{2}-E)^{\frac{3}{4}}(n+\frac{1}{2}-E)^{\frac{3}{4}}}.\end{aligned} \tag{2.12}$$

The scalar products inside the double series can be estimated using Wang's results on integrals of products of eigenfunctions of the harmonic oscillator [43]. While the scalar product clearly vanishes if $m+n=2s+1$, when both indices are either even or odd we get:

$$\begin{aligned}\langle\phi_{2m}\phi_0,\phi_0\phi_{2n}\rangle^2 \;&=\; \frac{1}{2\pi}\left[\frac{[2(m+n)]!}{(m+n)!}\right]^2\frac{1}{2^{4(m+n)}(2m)!(2n)!}\\ &\leq\; \frac{1}{2\pi}\left[\frac{[2(m+n)]!}{2^{2(m+n)}[(m+n)!]^2}\right]^2\\ &=\; \frac{\phi^4_{2(m+n)}(0)}{2},\end{aligned} \tag{2.13}$$

$$\begin{aligned}\left\langle\phi_{2m+1}\phi_0,\phi_0\phi_{2n+1}\right\rangle^2 \;&=\; \frac{1}{2\pi}\left[\frac{[2(m+n+1)]!}{(m+n+1)!}\right]^2\\ &\qquad\frac{1}{2^{4(m+n+1)}(2m+1)!(2n+1)!}\\ &\leq\; \frac{1}{2\pi}\left[\frac{[2(m+n+1)]!}{2^{2(m+n+1)}[(m+n+1)!]^2}\right]^2\\ &=\; \frac{\phi^4_{2(m+n+1)}(0)}{2},\end{aligned} \tag{2.14}$$

the final equalities in (2.13) and (2.14) resulting from Fassari and Inglese [44] and Mityagin and Siegl [45]. Therefore, the r.h.s. of (2.12) is bounded from above by:

$$\begin{aligned}\mathrm{tr}(\tilde{B}_E^2) \;\leq\; \frac{\pi^{\frac{3}{2}}}{8}\Bigg[&\sum_{m,n=0}^{\infty}\frac{\phi^4_{2(m+n)}(0)}{(2m+\frac{1}{2}-E)^{\frac{3}{4}}(2n+\frac{1}{2}-E)^{\frac{3}{4}}}\\ &+\sum_{m,n=0}^{\infty}\frac{\phi^4_{2(m+n+1)}(0)}{(2m+\frac{3}{2}-E)^{\frac{3}{4}}(2n+\frac{3}{2}-E)^{\frac{3}{4}}}\Bigg].\end{aligned} \tag{2.15}$$

As can be gathered from Mityagin and Siegl [45] using Stirling's formula,

$$\begin{aligned}\phi^4_{2n}(0) &\leq \frac{1}{\pi^2 n}, \quad n\geq 1,\\ \phi^4_{2(m+n)}(0) &\leq \frac{1}{\pi^2(m+n)}, \quad m,n\geq 1,\\ \phi^4_{2(m+n+1)}(0) &\leq \frac{1}{\pi^2(m+n+1)}, \quad m,n\geq 0,\end{aligned} \tag{2.16}$$

which implies that (2.15) is bounded by

$$\begin{aligned}\mathrm{tr}(\tilde{B}_E^2) \;\leq\;& \frac{1}{8\pi^{\frac{1}{2}}}\left[\frac{1}{(\frac{1}{2}-E)^{\frac{3}{2}}}+\frac{2}{(\frac{1}{2}-E)^{\frac{3}{4}}}\sum_{n=1}^{\infty}\frac{1}{n(2n+\frac{1}{2}-E)^{\frac{3}{4}}}\right]\\ &+\frac{1}{8\pi^{\frac{1}{2}}}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\frac{1}{m^{\frac{1}{2}}(2m+\frac{1}{2}-E)^{\frac{3}{4}}n^{\frac{1}{2}}(2n+\frac{1}{2}-E)^{\frac{3}{4}}}\\ &+\frac{1}{8\pi^{\frac{1}{2}}}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{1}{(m+\frac{1}{2})^{\frac{1}{2}}(2m+\frac{3}{2}-E)^{\frac{3}{4}}(n+\frac{1}{2})^{\frac{1}{2}}(2n+\frac{3}{2}-E)^{\frac{3}{4}}}\\ \leq\;& \frac{1}{8\pi^{\frac{1}{2}}}\left[\frac{1}{(\frac{1}{2}-E)^{\frac{3}{2}}}+\frac{2}{(\frac{1}{2}-E)^{\frac{3}{4}}}\sum_{n=1}^{\infty}\frac{1}{n^{\frac{1}{2}}(2n+\frac{1}{2}-E)^{\frac{3}{4}}}\right]\\ &+\frac{1}{8\pi^{\frac{1}{2}}}\left[\sum_{n=1}^{\infty}\frac{1}{n^{\frac{1}{2}}(2n+\frac{1}{2}-E)^{\frac{3}{4}}}\right]^2\\ &+\frac{1}{8\pi^{\frac{1}{2}}}\left[\sum_{n=0}^{\infty}\frac{1}{(n+\frac{1}{2})^{\frac{1}{2}}(2n+\frac{3}{2}-E)^{\frac{3}{4}}}\right]^2<\infty,\end{aligned} \tag{2.17}$$

since both series involved in the final expression are clearly absolutely convergent given that the summands are positive sequences decaying like $n^{-\frac{5}{4}}$. Hence, the trace of the square of the Birman-Schwinger operator, i.e., its Hilbert-Schmidt norm, is finite for any $E<\frac{1}{2}$.

Our result is not surprising at all since the norm could have been bounded by that of the Birman-Schwinger operator with the same impurity but with the resolvent of our H_0 replaced by that of $-\frac{\Delta}{2}$ in two dimensions, which is known to be finite [1]. However, it provides us with a far more accurate estimate of the norm, which in turn leads to a more precise determination of the spectral lower bound resulting from the use of the Hilbert-Schmidt norm of the Birman-Schwinger operator in the KLMN theorem [46]. In fact, the latter bound is what we wish to achieve by further estimating the bottom lines of (2.17).

The series in (2.17) can be bounded from above by their respective improper integrals as follows:

$$\begin{aligned} S_1 &= \sum_{n=1}^{\infty} \frac{1}{n^{\frac{1}{2}}(2n+\frac{1}{2}-E)^{\frac{3}{4}}} = \sum_{n=1}^{\infty} \frac{\sqrt{2}}{(2n)^{\frac{1}{2}}(2n+\frac{1}{2}-E)^{\frac{3}{4}}} \\ &< \int_0^{\infty} \frac{\sqrt{2}\,dx}{(2x)^{\frac{1}{2}}(2x+\frac{1}{2}-E)^{\frac{3}{4}}} \\ &= \frac{3\sqrt{2}}{4}\int_0^{\infty} \frac{s^{\frac{1}{2}}\,ds}{(s+\frac{1}{2}-E)^{\frac{7}{4}}} \leq \frac{3\sqrt{2}}{4}\int_0^{\infty} \frac{ds}{(s+\frac{1}{2}-E)^{\frac{5}{4}}} \\ &= \frac{3\sqrt{2}}{(\frac{1}{2}-E)^{\frac{1}{4}}}. \end{aligned} \tag{2.18}$$

$$\begin{aligned} S_2 &= \sum_{n=0}^{\infty} \frac{1}{(n+\frac{1}{2})^{\frac{1}{2}}(2n+\frac{3}{2}-E)^{\frac{3}{4}}} = \frac{\sqrt{2}}{(\frac{1}{2}-E)^{\frac{3}{4}}} \\ &+ \sum_{n=1}^{\infty} \frac{\sqrt{2}}{(2n+1)^{\frac{1}{2}}(2n+\frac{3}{2}-E)^{\frac{3}{4}}} \\ &< \frac{\sqrt{2}}{(\frac{1}{2}-E)^{\frac{3}{4}}} + \int_0^{\infty} \frac{\sqrt{2}\,dx}{(2x+1)^{\frac{1}{2}}(2x+\frac{3}{2}-E)^{\frac{3}{4}}} \\ &= \frac{\sqrt{2}}{(\frac{1}{2}-E)^{\frac{3}{4}}} - \frac{\sqrt{2}}{(\frac{1}{2}-E)^{\frac{3}{4}}} \\ &+ \frac{3\sqrt{2}}{4}\int_0^{\infty} \frac{(s+1)^{\frac{1}{2}}\,ds}{(s+\frac{3}{2}-E)^{\frac{7}{4}}} \leq \frac{3\sqrt{2}}{4}\int_0^{\infty} \frac{ds}{(s+\frac{3}{2}-E)^{\frac{5}{4}}} \\ &= \frac{3\sqrt{2}}{(\frac{3}{2}-E)^{\frac{1}{4}}}. \end{aligned} \tag{2.19}$$

Therefore, the bottom lines of (2.17) are bounded by:

$$\begin{aligned} \mathrm{tr}(\tilde{B}_E^2) &\leq \frac{1}{8\pi^{\frac{1}{2}}}\left[\frac{1}{(\frac{1}{2}-E)^{\frac{3}{2}}} + \frac{6\sqrt{2}}{\frac{1}{2}-E} + \frac{18}{(\frac{1}{2}-E)^{\frac{1}{2}}}\right] \\ &+ \frac{1}{8\pi^{\frac{1}{2}}}\frac{18}{(\frac{3}{2}-E)^{\frac{1}{2}}} \\ &= \frac{1}{8\pi^{\frac{1}{2}}(\frac{1}{2}-E)^{\frac{1}{2}}}\left[3\sqrt{2} + \frac{1}{(\frac{1}{2}-E)^{\frac{1}{2}}}\right]^2 \\ &+ \frac{1}{4\pi^{\frac{1}{2}}}\frac{9}{(\frac{3}{2}-E)^{\frac{1}{2}}}. \end{aligned} \tag{2.20}$$

Hence, our estimate of the Hilbert-Schmidt norm of the Birman-Schwinger operator is:

$$\begin{aligned} \mathrm{tr}(\tilde{B}_E^2) &= \left|\left| e^{-\frac{x^2+y^2}{2}}(H_0-E)^{-1}e^{-\frac{x^2+y^2}{2}} \right|\right|_2^2 \\ &\leq \frac{1}{8\pi^{\frac{1}{2}}(\frac{1}{2}-E)^{\frac{1}{2}}}\left[3\sqrt{2} + \frac{1}{(\frac{1}{2}-E)^{\frac{1}{2}}}\right]^2 + \frac{1}{4\pi^{\frac{1}{2}}}\frac{9}{(\frac{3}{2}-E)^{\frac{1}{2}}}. \end{aligned}$$

As is well known [22, 31, 32, 37, 38, 40, 41], the operator

$$(H_0-E)^{-1/2}e^{-(x^2+y^2)}(H_0-E)^{-1/2}$$

is isospectral to the Birman-Schwinger operator so that their Hilbert-Schmidt norms are identical. Hence, what has been achieved so far can be summarized by means of the following claim.

Theorem 2.1 *The integral operators*

$$(H_0-E)^{-1/2}e^{-(x^2+y^2)}(H_0-E)^{-1/2} \quad \textit{and} \quad e^{-\frac{x^2+y^2}{2}}(H_0-E)^{-1}e^{-\frac{x^2+y^2}{2}}$$

are Hilbert-Schmidt and their Hilbert-Schmidt norms satisfy

$$\begin{aligned} &\left|\left|(H_0-E)^{-1/2}e^{-(x^2+y^2)}(H_0-E)^{-1/2}\right|\right|_2^2 \\ &\qquad = \left|\left| e^{-\frac{x^2+y^2}{2}}(H_0-E)^{-1}e^{-\frac{x^2+y^2}{2}} \right|\right|_2^2 \\ &\leq \frac{1}{8\pi^{\frac{1}{2}}(\frac{1}{2}-E)^{\frac{1}{2}}}\left[3\sqrt{2} + \frac{1}{(\frac{1}{2}-E)^{\frac{1}{2}}}\right]^2 \\ &+ \frac{1}{4\pi^{\frac{1}{2}}}\frac{9}{(\frac{3}{2}-E)^{\frac{1}{2}}}. \end{aligned} \tag{2.21}$$

As an immediate consequence of the above theorem we get:

Corollary 1 *The Hamiltonian*

$$H_\lambda = H_0 - \lambda e^{-(x^2+y^2)},$$

defined in the sense of quadratic forms, is self-adjoint and bounded from below by E(λ), the solution of the equation:

$$\frac{1}{2(\frac{1}{2}-E)^{\frac{1}{2}}}\left[3\sqrt{2} + \frac{1}{(\frac{1}{2}-E)^{\frac{1}{2}}}\right]^2 + \frac{9}{(\frac{3}{2}-E)^{\frac{1}{2}}} = \frac{4\pi^{\frac{1}{2}}}{\lambda^2}. \tag{2.22}$$

Proof. For any $E < 0$ and $\psi \in Q(H_0) = D(H_0^{\frac{1}{2}})$ (the form domain of H_0):

$$\begin{aligned} &\lambda\left\langle \psi, e^{-(x^2+y^2)}\psi\right\rangle \\ &= \lambda\left\langle (H_0-E)^{1/2}\psi, \left[(H_0-E)^{-1/2}e^{-(x^2+y^2)}(H_0-E)^{-1/2}\right](H_0-E)^{1/2}\psi\right\rangle \\ &\leq \lambda\left|\left|(H_0-E)^{-1/2}e^{-(x^2+y^2)}(H_0-E)^{-1/2}\right|\right|_2 \left|\left|(H_0-E)^{1/2}\psi\right|\right|_2^2 \\ &\leq \lambda\left[\frac{1}{8\pi^{\frac{1}{2}}(\frac{1}{2}-E)^{\frac{1}{2}}}\left[3\sqrt{2} + \frac{1}{(\frac{1}{2}-E)^{\frac{1}{2}}}\right]^2 + \frac{1}{4\pi^{\frac{1}{2}}}\frac{9}{(\frac{3}{2}-E)^{\frac{1}{2}}}\right]^{\frac{1}{2}} \\ &\qquad \left[(\psi, H_0\psi) - E||\psi||_2^2\right]. \end{aligned} \tag{2.23}$$

By taking E sufficiently negative, the first factor in the bottom line of (2.23) can be made arbitrarily small, which ensures that the Gaussian perturbation is infinitesimally small with respect to H_0 in the sense of quadratic forms. Hence, we need only invoke the KLMN theorem (see [42]) to infer that H_λ is self-adjoint and bounded from below by the quantity

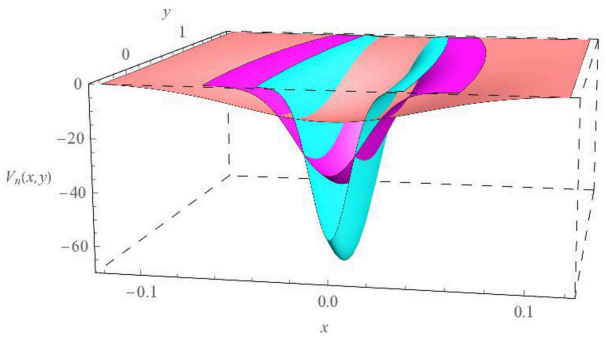

FIGURE 1 | Approximating potentials $V_n(x,y) = ne^{-(n^2x^2+y^2)}$ for $n = 15$ (pink), 30 (magenta), and 70 (cyan).

$$\frac{\lambda}{2\pi^{\frac{1}{4}}}\left[\frac{1}{2(\frac{1}{2}-E)^{\frac{1}{2}}}\left[3\sqrt{2}+\frac{1}{(\frac{1}{2}-E)^{\frac{1}{2}}}\right]^2+\frac{9}{(\frac{3}{2}-E)^{\frac{1}{2}}}\right]^{\frac{1}{2}} E, E<0, \tag{2.24}$$

so that the supremum of such lower bounds is attained for that particular value of E solving (2.22).

In the following subsections we first consider a Hamiltonian with a point interaction all along the x-direction in place of the Gaussian potential and then we investigate in detail the solution of (2.22), that is to say the lower bound of the spectrum of H_λ.

2.1. Hamiltonian With a Point Interaction Along the *x*-Direction

Let us consider now the Hamiltonian

$$H_\lambda^\delta = H_0 - \lambda\sqrt{\pi}\delta(x)e^{-y^2},$$

that is to say the energy operator given by the same H_0 as before but with the interaction term having a point interaction in place of the Gaussian along the x-direction. Our goal is to prove that such an operator is self-adjoint and that it is the limit in the norm resolvent sense of the sequence $H_0 - \lambda V_n(x,y)$ as $n \to \infty$, with $V_n(x,y) = ne^{-(n^2x^2+y^2)}$. As is to be expected, our approximating sequence is quite different from the one used in Albeverio et al. [1] to get the Laplacian perturbed by a point interaction in two dimensions. Before stating and proving the main result of this section, we wish to provide the reader with the visualization of the approximating potentials in **Figure 1**.

Corollary 2 *The Hamiltonian $H_\lambda^\delta = H_0 - \lambda\sqrt{\pi}\delta(x)e^{-y^2}$, defined in the sense of quadratic forms, is self-adjoint and is the norm resolvent limit of the sequence of Hamiltonians*

$$H_{n,\lambda} = H_0 - \lambda ne^{-(n^2x^2+y^2)}.$$

Furthermore, H_λ^δ is bounded from below by $E_\delta(\lambda)$, the solution of the equation:

$$\frac{1}{(\frac{1}{2}-E)^{\frac{1}{2}}}\left[\frac{1}{(\frac{1}{2}-E)^{\frac{1}{2}}}+3\sqrt{2}\right]^2 = \frac{4\pi^{\frac{1}{2}}}{\lambda^2}. \tag{2.25}$$

Proof. First of all, it is quite straightforward to show that the integral operator

$$(H_0-E)^{-1/2}\sqrt{\pi}\delta(x)e^{-y^2}(H_0-E)^{-1/2}, \quad E<0,$$

is Hilbert-Schmidt with the square of the Hilbert-Schmidt norm given by:

$$\begin{aligned}
&\pi\left|\left|(H_0-E)^{-1/2}\delta(x)e^{-y^2}(H_0-E)^{-1/2}\right|\right|_2^2\\
&=\pi\left|\left|(\delta(x)e^{-y^2})^{\frac{1}{2}}(H_0-E)^{-1}(\delta(x)e^{-y^2})^{\frac{1}{2}}\right|\right|_2^2\\
&=\pi\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{-y^2}e^{-y'^2}\left[(H_0-E)^{-1}(0,0,y,y')\right]^2dydy'\\
&=\pi\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{-y^2}e^{-y'^2}\left[\sum_{n=0}^{\infty}\frac{e^{-\sqrt{2(2n+\frac{1}{2}-E)}|y'-y''|}}{\sqrt{2\left(2n+\frac{1}{2}-E\right)}}\phi_{2n}^2(0)\right]^2dydy'\\
&=\frac{\pi}{2}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\phi_{2m}^2(0)\phi_{2n}^2(0)\\
&\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{-y^2}\frac{e^{-\sqrt{2(2m+\frac{1}{2}-E)}|y-y'|}e^{-\sqrt{2(2n+\frac{1}{2}-E)}|y-y'|}}{\sqrt{\left(2m+\frac{1}{2}-E\right)\left(2n+\frac{1}{2}-E\right)}}e^{-y'^2}dydy'.
\end{aligned}$$

As the double integral involving the convolution has already been estimated in (2.11), the latter expression is bounded by:

$$\begin{aligned}
&\frac{\pi^{3/2}}{4}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{\phi_{2m}^2(0)\phi_{2n}^2(0)}{(2m+\frac{1}{2}-E)^{\frac{3}{4}}(2n+\frac{1}{2}-E)^{\frac{3}{4}}}\\
&\qquad=\frac{\pi^{3/2}}{4}\left[\sum_{n=0}^{\infty}\frac{\phi_{2n}^2(0)}{(2n+\frac{1}{2}-E)^{\frac{3}{4}}}\right]^2,
\end{aligned} \tag{2.26}$$

which, using (2.17), is bounded by:

$$\begin{aligned}
&\frac{1}{4\pi^{1/2}}\left[\frac{1}{(\frac{1}{2}-E)^{\frac{3}{4}}}+\sum_{n=1}^{\infty}\frac{1}{n^{\frac{1}{2}}(2n+\frac{1}{2}-E)^{\frac{3}{4}}}\right]^2\\
&\quad\le\frac{1}{4\pi^{1/2}}\left[\frac{1}{(\frac{1}{2}-E)^{\frac{3}{4}}}+\frac{3\sqrt{2}}{(\frac{1}{2}-E)^{\frac{1}{4}}}\right]^2\\
&\qquad=\frac{1}{4\pi^{\frac{1}{2}}(\frac{1}{2}-E)^{\frac{1}{2}}}\left[\frac{1}{(\frac{1}{2}-E)^{\frac{1}{2}}}+3\sqrt{2}\right]^2,
\end{aligned} \tag{2.27}$$

having taken advantage of (2.18). As the right hand side of (2.27) can be made arbitrarily small by taking $E < 0$ large in absolute value, the KLMN theorem ensures, as was done previously in the case of H_λ, the self-adjointness of H_λ^δ as well as the existence of the spectral lower bound $E_\delta(\lambda)$ given by the solution of (2.25).

As to the convergence of $H_{n,\lambda}$ to H_λ^δ, we start by noting that, for any $E < 0$, the operator $(H_0-E)^{-1/2}ne^{-(n^2x^2+y^2)}(H_0-E)^{-1/2}$

converges weakly to $(H_0 - E)^{-1/2}\sqrt{\pi}\delta(x)e^{-y^2}(H_0 - E)^{-1/2}$ as $n \to \infty$. Furthermore,

$$\begin{aligned}
&\left|\left|(H_0 - E)^{-1/2} n e^{-(n^2x^2+y^2)}(H_0 - E)^{-1/2}\right|\right|_2^2 \\
&= \left|\left| n e^{-\frac{n^2x^2+y^2}{2}}(H_0 - E)^{-1} e^{-\frac{n^2x^2+y^2}{2}} \right|\right|_2^2 \\
&= \sum_{l,m=0}^{\infty}\left[\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-y^2}\frac{e^{-\left(\sqrt{2(l+\frac{1}{2}-E)}+\sqrt{2(m+\frac{1}{2}-E)}\right)|y-y'|}}{2\sqrt{(l+\frac{1}{2}-E)(m+\frac{1}{2}-E)}} e^{-y'^2} dy dy'\right] \\
&\quad \left\langle \phi_l, n e^{-n^2(\cdot)^2}\phi_m\right\rangle^2. \qquad (2.28)
\end{aligned}$$

Since

$$\begin{aligned}
\left\langle \phi_l, n e^{-n^2(\cdot)^2}\phi_m\right\rangle &= n\int_{-\infty}^{\infty} e^{-n^2x^2}\phi_l(x)\phi_m(x)dx \\
&= \int_{-\infty}^{\infty} e^{-x^2}\phi_l(x/n)\phi_m(x/n)dx \to \sqrt{\pi}\phi_l(0)\phi_m(0),
\end{aligned}$$

as $n \to \infty$, the right hand side of (2.28) converges to

$$\begin{aligned}
&\frac{\pi}{2}\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}\phi_{2l}^2(0)\phi_{2m}^2(0) \\
&\left[\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-y^2}\frac{e^{-\left(\sqrt{2(2l+\frac{1}{2}-E)}+\sqrt{2(2m+\frac{1}{2}-E)}\right)|y-y'|}}{\sqrt{(2l+\frac{1}{2}-E)(2m+\frac{1}{2}-E)}} e^{-y'^2} dy dy'\right] \\
&= \pi\left|\left|(\delta(x)e^{-y^2})^{\frac{1}{2}}(H_0 - E)^{-1}(\delta(x)e^{-y^2})^{\frac{1}{2}}\right|\right|_2^2 \\
&= \pi\left|\left|(H_0 - E)^{-1/2}\delta(x)e^{-y^2}(H_0 - E)^{-1/2}\right|\right|_2^2.
\end{aligned}$$

Hence, the Hilbert-Schmidt norm of $(H_0 - E)^{-1/2} n e^{-(n^2x^2+y^2)}(H_0 - E)^{-1/2}$ converges to the Hilbert-Schmidt norm of $(H_0 - E)^{-1/2}\sqrt{\pi}\delta(x)e^{-y^2}(H_0 - E)^{-1/2}$ as $n \to \infty$. Due to Theorem 2.21 in Simon [47], this fact and the previous weak convergence imply that the convergence actually takes place in the Hilbert-Schmidt norm. Then, the norm convergence of these integral operators ensures the norm resolvent convergence of $H_{n,\lambda}$ to H_λ^δ, as guaranteed by Theorem VIII.25 in Reed and Simon [46], which completes our proof of Corollary 2.

2.2. The Lower Bound of $\sigma(H_0 - \lambda e^{-(x^2+y^2)})$

As anticipated earlier, the lower bound of the spectrum of H_λ in (1.3) is the function $E(\lambda)$ given implicitly by the equation (2.22). From this expression, some approximate results can be easily obtained in two different regimes. For example, it is possible to prove that the asymptotic behavior of (2.22) for large values of both variables $E(\lambda), \lambda$ is

$$E(\lambda) = -\frac{81}{4\pi^2}\lambda^4. \qquad (2.29)$$

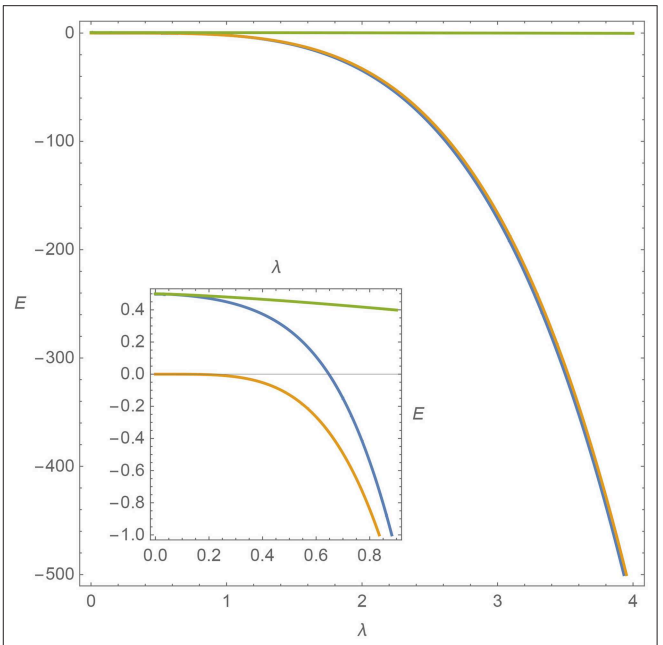

FIGURE 2 | A plot of the lower bound of the energy E as a function of λ resulting from the solution of Equation (2.22) (blue curve), the approximate expression valid for large values of E and λ obtained in (2.29) (yellow curve) and the approximation for small values of λ as in (2.30) (green curve). In the inset we have enlarged the region where λ and E are small. While the similarity between the solution of (2.22) and the funtion (2.29) is quite acceptable for a wide range of the parameters, the solution of (2.22) is satisfactorily approximated by (2.30) only for very small values of λ.

On the other hand, for small values of λ we can prove that (2.22) behaves approximately as follows

$$E(\lambda) = \frac{1}{2} - \frac{1}{4\pi^{2/3}}\lambda^{4/3}. \qquad (2.30)$$

A plot of the λ-dependence (λ being the strength of the potential of H_λ) of the lower bound of the energy $E(\lambda)$, resulting from the solution of (2.22), as well as those of the two approximations given by (2.29) and (2.30), are given in **Figure 2**.

3. FINAL REMARKS

In this note we have analyzed in detail the Birman-Schwinger operator of the two-dimensional Hamiltonian $H_\lambda = H_0 - \lambda e^{-(x^2+y^2)}$, namely the integral operator $-\lambda e^{-\frac{x^2+y^2}{2}}(H_0 - E)^{-1}e^{-\frac{x^2+y^2}{2}}$ where $H_0 = (-\frac{1}{2}\frac{d^2}{dx^2} + \frac{x^2}{2}) - \frac{1}{2}\frac{d^2}{dy^2}$. In particular, we have rigorously shown that the operator is Hilbert-Schmidt and have estimated its Hilbert-Schmidt norm. This fact has enabled us to use the KLMN theorem to determine a lower bound for the spectrum of H_λ, that is to say $E(\lambda)$, the implicit function representing the solution of an equation involving the energy parameter and the coupling constant. Furthermore, we have investigated the Hamiltonian $H_\lambda^\delta = H_0 - \lambda\sqrt{\pi}\delta(x)e^{-y^2}$, having the Gaussian impurity in the direction subjected to the harmonic confinement replaced by a point impurity.

As anticipated in the introduction, the proof of the resolvent convergence, as the thickness of the layer vanishes, of the Hamiltonian of a three-dimensional parabolic quantum well inside a thin layer to the 2D Hamiltonian (1.3) has been put off as it may deserve a separate paper.

The results of this article will enable us to study the lowest bound states created by the Gaussian impurity potential of the aforementioned Hamiltonian by means of the modified Fredholm determinant $\det_2\left[1-\lambda e^{\frac{x^2+y^2}{2}}(H_0-E)^{-1}e^{-\frac{x^2+y^2}{2}}\right]$, the regularized determinant used to handle Hilbert-Schmidt operators. Work in this direction is in progress.

DATA AVAILABILITY

All datasets generated for this study are included in the manuscript and/or the supplementary material.

AUTHOR CONTRIBUTIONS

All authors listed have made a substantial, direct and intellectual contribution to the work, and approved it for publication.

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One-Dimensional Scattering of Fermions on δ-Impurities

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We study the spectrum of the 1D Dirac Hamiltonian encompassing the bound and scattering states of a fermion distorted by a static background built from δ-function potentials. After introducing the most general Dirac-δ potential for the Dirac equation we distinguish between "mass-spike" and "electrostatic" δ-potentials. Differences in the spectra arising depending on the type of δ-potential are studied in deep detail.

Keywords: contact interactions, Dirac equation, Dirac delta, selfadjoint extensions, relativistic quantum mechanics

1. INTRODUCTION

The Dirac equation with various relativistic potentials mimicking string-like or vortex-like backgrounds has a long history. The best known example is the Aharonov-Bohm [1] interaction of charged fermions with a field of an infinitesimally thin solenoid. The scattering of fermions on magnetic 'tHooft-Polyakov monopoles and on Abrikosov-Nielsen-Olesen strings with consequent fractional fermion numbers and fermion number non-conservation was a hot topic in the late 70s and early 80s [2, 3]. The cosmic strings predicted by grand unified theories also appeared to interact with fermions (matter) via the Aharonov-Bohm mechanism [4]. The non-relativistic limit of the scattering problem for spin-one-half particles in the Aharonov-Bohm potential in (1+2) conical space was examined in [5, 6].

It was observed that in the case of a point magnetic vortex (Aharonov-Bohm interaction) one can either with gauge transformation reduce the problem to a Laplace equation with delta-potential or to a free Dirac equation with a special angular boundary condition [7]. A radial boundary condition specifies the self-adjoint extension. From the operator theory viewpoint the Dirac operator with relativistic point interaction (δ-function potentials) and its self-adjoint extensions were considered in [8, 9]. In the last years the low-dimensional problems of this kind were investigated topologically with the Levinson theorem, which proved to be closely related to an index theorem [10].

A renewed interest to Dirac equation with singular potentials was inspired by the appearance of the new 2D materials. Graphene in the field of a Aharonov-Bohm solenoid perpendicular to its plane was considered in [11]. The induced current and induced charge density were calculated. Another example is a magnetic Kronig-Penney model for Dirac electrons in single-layer graphene developed in [12]. The model is a series of very high and very narrow magnetic δ-function barriers alternating in sign.

In this paper we describe the distortion caused by impurities in the free propagation of fermionic fields in the $1+1$-dimensional Minkowski spacetime by means of Dirac δ-point interactions. We elaborate on and develop further previous work on this subject in References [13, 14]. The matching conditions appropriated to define the δ-potential inserted in a Dirac Hamiltonian restricted to a line were proposed some time ago in References [15, 16].

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Our aim is to generalize the study carried out in References [17–19] to fermionic fields so that we can use the results in effective QFT models of 2D materials.

Throughout the paper we shall use natural units where $\hbar = c = 1$ (henceforth, $L = T = M^{-1}$). In addition we will fix the Minkowski spacetime metric tensor to be: $\eta^{\mu\nu} \equiv \text{diag}(+,-)$. Having done these choices, the Hamiltonian form of the Dirac equation, governing the dynamics of a free fermionic particle of mass m moving on a line, reads

$$i\partial_t\psi(t,x) = \boldsymbol{H}_D^{(0)}\psi(t,x) = [-i\alpha\partial_x + \beta m]\psi(t,x), \qquad (1)$$

or, in covariant form:

$$(i\gamma^\mu\partial_\mu - m\,)\psi(x) = 0.$$

For the fermionic anti-particle the dynamics is governed by the conjugate Dirac Hamiltonian

$$i\partial_t\phi(t,x) = \overline{\boldsymbol{H}}_D^{(0)}\phi(t,x) = [-i\alpha\partial_x - \beta m]\phi(t,x), \qquad (2)$$

or, in covariant form

$$(i\gamma^\mu\partial_\mu + m\,)\phi(x) = 0.$$

Here, the $\{\gamma^\mu\}_{\mu=0,1}$ matrices close the Clifford algebra of $\mathbb{R}^{1,1}$ that can be minimally represented by "pseudo-Hermitian"two-by-two matrices: $\gamma^{\mu\,\dagger} = \gamma^0\gamma^\mu\gamma^0$. Explicitly,

$$\{\gamma^\mu,\gamma^\nu\} \equiv \gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2\eta^{\mu\nu} \;\Rightarrow$$
$$\gamma^0\gamma^0 = \mathbb{1} = -\gamma^1\gamma^1\,,\;\; \gamma^0\gamma^1 = -\gamma^1\gamma^0.$$

We shall need also the 1+1-dimensional analogue of the γ^5 matrix, denoted throughout this paper as γ^2:

$$\gamma^2 = \gamma^0\gamma^1.$$

The free Dirac Hamiltonians appearing in the formulas (1)–(2) demand thus the definition of the α and β Dirac matrices:

$$\beta = \gamma^0, \qquad \alpha = \gamma^0\gamma^1 = \gamma^2.$$

In order to perform explicit calculations we shall stick to the following choice of γ-matrices:

$$\gamma^0 = \sigma_3 = \beta, \qquad \gamma^1 = i\sigma_2, \qquad \gamma^2 = \sigma_1 = \alpha, \qquad (3)$$

where $\sigma_1, \sigma_2, \sigma_3$ are the Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Our choice of gamma matrices enables us to identify the three discrete transformations acting on the Dirac spinors:

1. Parity transformation $\mathcal{P}$: $\mathcal{P}\psi(x,t) = (-1)^p\gamma^0\psi(-x,t)$, where $p = 0, 1$, is the intrinsic parity of the particle
2. Time-reversal transformation $\mathcal{T}$: $\mathcal{T}\psi(x,t) = \gamma^0\psi^*(x,-t)$.
3. Charge conjugation transformation $\mathcal{C}$: $\mathcal{C}\psi(x,t) = \gamma^2\psi^*(x,t)$.

Parity and time-reversal are symmetries of the free Dirac Hamiltoninan (1) and its conjugate (2). Charge conjugation, however, transforms the free Dirac Hamiltonian into its conjugate and viceversa. This property is the secret behind the common wisdom in Fermi field theory where negative energy fermions are traded by positive energy antifermions. More precisely: both $\boldsymbol{H}_D^{(0)}$ and $\overline{\boldsymbol{H}}_D^{(0)}$ have a Dirac sea of negative energy states. The idea is to form a complete set of spinors from the positive energy states of $\boldsymbol{H}_D^{(0)}$, fermions, and the positive energy eigen spinors of $\overline{\boldsymbol{H}}_D^{(0)}$, anti-fermions. In this spirit one checks that the solutions for the conjugate Dirac equation are related to the solutions of the Dirac equation by the charge conjugation transformation. Given the spectral problems

$$\boldsymbol{H}_D^{(0)}\psi_\omega(x) = \omega\psi_\omega(x), \quad \overline{\boldsymbol{H}}_D^{(0)}\phi_\omega(x) = \omega\phi_\omega(x), \qquad (4)$$

the eigenspinors are related through charge conjugation: $\phi_\omega = \gamma^2\psi_\omega^*(x)$. Equivalently, one finds that: $\mathcal{C}\boldsymbol{H}_D^{(0)}\mathcal{C}^{-1} = \overline{\boldsymbol{H}}_D^{(0)}$.

Consider next a bunch of relativistic Fermi particle propagating in (1+1)D Minkowski spacetime under the influence of a external time-independent classical background. The most general Dirac Hamiltonian describing this situation reads:

$$\boldsymbol{H}_D = \boldsymbol{H}_0 + V(x) = -i\alpha\partial_x + \beta m + V(x). \qquad (5)$$

The external potential comprises four types (see [14]):

$$V(x) = V_0(x)\mathbb{1} + V_1(x)\alpha + V_2(x)\beta + V_3(x)\alpha\beta. \qquad (6)$$

In Ref. [14], it is shown that:

- It is possible to assume $V_1(x) = 0$ without loss of generality since it can be absorbed by a gauge transformation.
- It is convenient to choose $V_3(x) = 0$ to avoid interactions of the type $\bar\psi\gamma^2V_3(x)\psi$ which are only consistent if V_3 is purely imaginary.

Hence, we shall focus our attention on background potentials of the form

$$V(x) = \xi(x)\,\mathbb{1} + M(x)\beta, \qquad (7)$$

leading to the following Dirac spectral problem

$$\begin{aligned}\boldsymbol{H}_D\psi(x) \;&=\; \omega\psi(x) \;\Rightarrow\; [-i\alpha\partial_x + \beta(m + M(x))]\psi(x)\\ &=\; [\omega - \xi(x)]\psi(x).\end{aligned} \qquad (8)$$

In formula (8) the $\xi(x)$ potential clearly appears as an electrostatic potential, whereas the potential energy $M(x)$ shows itself as a position dependent mass. Note that this last potential can be reinterpreted as an interaction of the Dirac field with a classical scalar field. Different elections for the electrostatic potential $\xi(x)$, and the mass-like potential $M(x)$ have been done in the last two decades: in Ref. [20] it is studied the choice of $\xi(x)$ and $M(x)$ as Coulomb and quadratic *vetor potentials*, and and in Refs. [21, 22]

the possibility of $\xi(x)$ and $M(x)$ being quadratic, linear, and other confining potentials is considered.

We shall focus on external potentials localized in one point meaning that the propagating fermion finds an impurity at that point. Analytically we mimic the influence of the impurity on the fermion by a δ-function potential. We thus choose:

$$V(x) = \Gamma(q,\lambda)\delta(x); \quad \Gamma(q,\lambda) = q\mathbb{1} + \lambda\beta. \tag{9}$$

It is of note that the weight term $\Gamma(q,\lambda)$ multiplying the $\delta(x)$-function in formula (9) is a 2×2 matrix depending on two coupling constants: physically q plays the role of a dimensionless electric charge[1] and λ is also non dimensional, but plays the role of a scalar or gravitational coupling because it couples to the Fermi fields like a mass. Physically all this enables to interpret the most general form of the delta potential as a point charge plus a variable mass, in parallel to that taken in [17] devoted to scalar field interactions with external δ-plates.

Early distributional definitions of δ-point interaction for Dirac fields were proposed in Refs. [15, 16]. In these references, the purely electrostatic fermionic Dirac-δ potential was defined through a matching condition of the form

$$\psi(0^+) = T_{E\delta}(q)\psi(0^-); \quad T_{E\delta}(q) = \mathbb{1}\cos(q) - i\gamma^2\sin(q). \tag{10}$$

Later, in Ref. [14] the matching condition (10) was extended for the general δ-potential (9), following the approach of [16], to be:

$$\psi(0^+) = T_\delta(q,\lambda)\psi(0^-); \quad T_\delta(q,\lambda) = \exp\left(-i\gamma^2\Gamma(q,\lambda)\right) \tag{11}$$
$$T_\delta(q,\lambda) = \mathbb{1}\cos\Omega - \frac{i}{2}\sin\Omega\left[\frac{\Omega}{q+\lambda}(\gamma^2+\gamma^1) + \frac{q+\lambda}{\Omega}(\gamma^2-\gamma^1)\right],$$

being $\Omega = \sqrt{q^2-\lambda^2}$. It is straightforward to obtain the matrix that defines the mass-spike Dirac-δ potential:

$$T_{M\delta}(\lambda) = T_\delta(0,\lambda) = \mathbb{1}\cosh(\lambda) + i\gamma^1\sinh(\lambda). \tag{12}$$

This last particular case is what is studied in detail in Ref. [14] regarding the Casimir effect induced by vacuum fermionic quantum fluctuations.

In order to comprehend the results of the calculations in the following sections it is convenient to take into account the transformation properties of the point-supported potential defined by equation (11) under parity ($\mathcal{P}$), time-reversal ($\mathcal{T}$), and charge conjugation ($\mathcal{C}$).

- Taking into account that the parity-transformed spinor $\psi^P \equiv \mathcal{P}\psi$ satisfies

  $$\psi^P(0^\pm) = \gamma^0\psi(0^\mp),$$

  the matching condition $\psi^P(0^+) = T^P_\delta(q,\lambda)\psi^P(0^-)$ is automatically satisfied:

  $$T^P_\delta(q,\lambda) \equiv \gamma^0 T_\delta(q,\lambda)^{-1}\gamma^0 = T_\delta(q,\lambda). \tag{13}$$

  Thus, (13) guarantees that $T_\delta(q,\lambda)$ remains invariant under parity transformation such that the general fermionic δ-potential is parity invariant, as it happens in the bosonic case.
- Denoting $\psi^T(x,t) \equiv \mathcal{T}\psi(x,t)$, the matching condition (11) imposes over ψ^T the time-reversal transformed matching conditon

  $$\psi^T(0^+) = T^T_\delta(q,\lambda)\psi^T(0^-); \quad T^T_\delta(q,\lambda) = \gamma^0 T_\delta(q,\lambda)^*\gamma^0. \tag{14}$$

  One immediately realizes that $T^T_\delta(q,\lambda) = T_\delta(q,\lambda)$. Hence the fermionic δ-potential maintains the time-reversal invariance as in the scalar case.
- The charge conjugated spinors $\psi^C \equiv \mathcal{C}\psi$ must satisfy the conjugated matching conditions:

  $$\psi^C(0^+) = T^C_\delta(q,\lambda)\psi^C(0^-), \tag{15}$$

  where the charge-conjugated matching matrix is:

  $$T^C_\delta(q,\lambda) = \gamma^2 T_\delta(q,\lambda)^*\gamma^2 = T_\delta(-q,\lambda). \tag{16}$$

  Thus, the fermionic δ-potential as defined in (11) is not invariant under charge conjugation changing q by $-q$ as long as $q \neq 0$. This result is what one expects implicitly considering the term with the coupling q in (11) as an electrostatic potential [14].

Therefore, we are led to solve simultaneously the spectral problems for the Dirac Hamiltonian and its conjugate together with the δ-matching condition and its conjugate:

$$\boldsymbol{H}^{(0)}_D\psi(x) = \omega\psi(x); \quad \psi(0^+) = T_\delta(q,\lambda)\psi(0^-), \tag{17}$$
$$\overline{\boldsymbol{H}}^{(0)}_D\phi(x) = \omega\phi(x); \quad \phi(0^+) = T_\delta(-q,\lambda)\phi(0^-). \tag{18}$$

The eigenspinors of $\boldsymbol{H}^{(0)}_D$ with $\omega > m$ obeying the matching condition in (17) correspond to electron scattering states, whereas those with $-m < \omega < m$ refer to electron bound states. On the contrary, the $\overline{\boldsymbol{H}}^{(0)}_D$ eigenspinors with $\omega > m$ complying with the matching condition in (18) can be treated as positron scattering states, but those with $-m < \omega < m$ we attribute to positron bound states.

The main objective of the present work is the study of this spectral problem in $1D$ relativistic quantum mechanics in order to build a fermionic quantum field theory system where the one-particle/antiparticle states are the eigenstates of $\boldsymbol{H}_D/\overline{\boldsymbol{H}}^{(0)}_D$. The fermionic Fock space is thus constructed from these eigenstates instead of plane waves. In the next Section we introduce the necessary notation and basic formulas to understand the behavior of fermions in a flat background without any external potential. In section 3 we consider the dynamics of a relativistic 1D Fermi particle and antiparticle in one electrostatic δ-potential $V = q\delta(x)\mathbb{1}$ describing the effect of one impurity on the free propagation. Fermions (antifermions) are either trapped in bound states or distorted in scattering waves of $\boldsymbol{H}_D$ ($\overline{\boldsymbol{H}}_D$). The charge density of the bound states is also computed. In section 4, the same study is performed for a mass-spike delta potential $V = \lambda\delta(x)\sigma_3$. A summary and outlook are offered in the last section.

[1] We shall allow q to vary as an angle proportional to the fine structure constant, which in a $1D$ space is $\alpha = |\frac{e^2}{m^2}|$, the electron charge times the Compton particle wavelength to the square.

2. ELECTRON/POSITRON PROPAGATION ON A LINE

We consider the one-dimensional Dirac field

$$\Psi(t,x)=\begin{pmatrix}\psi_1(t,x)\\ \psi_2(t,x)\end{pmatrix};\ \psi_1(t,x):\mathbb{R}^{1,1}\to\mathbb{C},\ \psi_2(t,x):\mathbb{R}^{1,1}\to\mathbb{C},$$

and set the following Dirac action:

$$S_D=\int dt\int dx\left\{\bar{\Psi}(t,x)\left(i\gamma^\mu\partial_\mu-m\right)\Psi(t,x)\right\},\quad(19)$$

in the Dirac representation of the Clifford algebra taking into account our choice of γ matrices. In the natural system of units, the dimension of the Dirac field Ψ is: $[\Psi]=L^{-1/2}$. The Euler-Lagrange equation derived from the action (19) is the Dirac equation

$$\begin{gathered}i\sigma_3\partial_t\Psi=\sigma_2\partial_x\Psi+m\Psi,\quad(20)\\ \begin{pmatrix}i\partial_t-m & i\partial_x\\ -i\partial_x & -i\partial_t-m\end{pmatrix}\begin{pmatrix}\psi_1(t,x)\\ \psi_2(t,x)\end{pmatrix}=\begin{pmatrix}0\\0\end{pmatrix}.\end{gathered}$$

The time-energy Fourier transform

$$\psi_1(t,x)=\int d\omega\, e^{-i\omega t}\,\psi_1^\omega(x),\qquad \psi_2(t,x)=\int d\omega\, e^{-i\omega t}\,\psi_2^\omega(x),$$

reduces the PDE Dirac equation to the ODE system

$$(\omega-m)\psi_1^\omega(x)+i\frac{d\psi_2^\omega}{dx}=0\quad,\quad i\frac{d\psi_1^\omega}{dx}+(\omega+m)\psi_2^\omega(x)=0.\quad(21)$$

It is clear that the system (21) is no more than the spectral equation for the quantum mechanical free Dirac Hamiltonian:

$$\boldsymbol{H}_0\Psi^\omega(x)=\omega\Psi^\omega(x)\,,\boldsymbol{H}_0=-i\sigma_1\frac{d}{dx}+m\sigma_3=\begin{pmatrix}m & -i\frac{d}{dx}\\ -i\frac{d}{dx} & -m\end{pmatrix},$$

acting on time-independent spinors[2]. We remark now that a similar strategy based on time-energy Fourier transform also works when the effect of an external static potential, like those mentioned in the Introduction, is included in the action. The only required modification is to replace $\boldsymbol{H}_0$ by $\boldsymbol{H}_D$.

The analysis of free propagation also admits a position-momentum Fourier transform:

$$\psi_1^\omega(x)=\int dk\,A(k)e^{ikx},\qquad \psi_2^\omega(x)=\int dk\,B(k)e^{ikx},$$

which converts the ODE system (21) in the algebraic homogeneous system

$$(\omega-m)\,A(k)-k\,B(k)=0,\qquad k\,A(k)-(\omega+m)\,B(k)=0.\quad(22)$$

[2]We shall refer as spinor fields to the Fermi fields even though in one-dimension there is no spin.

Introducing the positive and negative energy eigenspinors which satisfy (22) with $k=0$,

$$\Psi^+(t,x)=A\begin{pmatrix}e^{-imt}\\0\end{pmatrix},\qquad \Psi^-(t,x)=B\begin{pmatrix}0\\e^{+imt}\end{pmatrix},$$

it is easy to derive the non-trivial solutions of (22).

They occur if the following spectral condition holds

$$\det\begin{pmatrix}\omega-m & -k\\ k & -(\omega+m)\end{pmatrix}=0\ \equiv\ \omega=\omega_\pm=\pm\sqrt{k^2+m^2},$$

and the eigenspinors of moving electrons split in two types:
(1) Positive energy ω_+ electron spinor plane waves moving along the real axis with momentum $k\in\mathbb{R}$. The solution of (22), $B(k)=k/(\omega_++m)A(k)$, implies that the positive energy eigenspinors are

$$\Psi^+(t,x;k)=\!A\,e^{-i\omega_+t}e^{ikx}\,u_+(k)\ ,\ \ u_+(k)=\begin{pmatrix}1\\ \frac{k}{\omega_++m}\end{pmatrix}.\quad(23)$$

(2) Negative energy ω_- electron spinor plane waves moving along the real axis with momentum $k\in\mathbb{R}$. We choose the solution $A(k)=k/(\omega_--m)B(k)$ of (22) to find the negative energy eigenspinors

$$\Psi^-(t,x;k)=\!B\,e^{-i\omega_-t}e^{ikx}u_-(k)\ ,\ \ u_-(k)=\begin{pmatrix}\frac{k}{\omega_--m}\\ 1\end{pmatrix}.\quad(24)$$

In 1D space the concept of the holes in the Dirac sea is implemented by replacing the negative energy spinors $u_-(k)$ with the positron spinors,

$$v_+(k)=\gamma^2u_+^*(k)=\begin{pmatrix}\frac{k}{\omega_++m}\\ 1\end{pmatrix}.\quad(25)$$

which are solutions of the conjugated Dirac equation:

$$(\omega+m)\phi_1^\omega(x)+i\frac{d\phi_2^\omega}{dx}=0\quad,\quad i\frac{d\phi_1^\omega}{dx}+(\omega-m)\phi_2^\omega(x)=0\ .\quad(26)$$

Note that the $v_+(k)$ spinors are also orthogonal to the positive energy spinors $u_+(k)$. We thus describe the propagation of 1D fermions in terms of electron and positron plane waves:

$$\begin{aligned}&\psi_k^+\ \propto\ u_+(k)e^{ikx}e^{-i\omega_+t}\quad\text{electron with momentum } k\text{, energy }\omega_+\\ &\phi_k^+\ \propto\ v_+(k)e^{ikx}e^{-i\omega_+t}\quad\text{positron with momentum } k\text{, energy }\omega_+\end{aligned}$$

Therefore, from now on, we will work with the bihamiltonian system given in (17-18), where the positron energy and the electron energy are always chosen as $\omega=+\sqrt{k^2+m^2}$.

3. "ELECTROSTATIC"POINT DELTA-INTERACTION

Consider now a relativistic 1D fermion whose free propagation is disturbed by one impurity concentrated in one point

that we describe by including a δ-potential. The one-dimensional Dirac Hamiltonian with a single Dirac δ-potential of "electrostatic"type is:

$$H_{\mathrm{E}\delta} = -i\sigma_1\frac{d}{dx} + m\sigma_3 + q\delta(x)\mathbb{1}, \quad q = \nu\frac{e^2}{m^2} \in \mathbb{S}^1,$$
$$\nu \in (0, 2\pi\frac{m^2}{e^2}).$$

Recall that q is dimensionless: $[q] = 1$. The spectral equation for this Hamiltonian $H_{\mathrm{E}\delta}\Psi(x) = \omega\Psi(x)$ is equivalent to the Dirac system of two first-order ODE's:

$$-i\frac{d\psi_2}{dx} = (\omega - m)\psi_1(x), \tag{27}$$
$$-i\frac{d\psi_1}{dx} = (\omega + m)\psi_2(x), \tag{28}$$

where the eigenspinors for the free Dirac Hamiltonian in zone I ($x < 0$) and those in zone II ($x > 0$), must be related across the singularity at $x = 0$ by the "electrostatic"matching conditions defined in (10):

$$\begin{pmatrix}\psi_1(0^+)\\ \psi_2(0^+)\end{pmatrix} = \begin{pmatrix}\cos q & -i\sin q\\ -i\sin q & \cos q\end{pmatrix}\begin{pmatrix}\psi_1(0^-)\\ \psi_2(0^-)\end{pmatrix}. \tag{29}$$

Similarly, positron propagation disturbed by impurities that can be studied through $\overline{H}_{\mathrm{E}\delta}\Phi(x) = \omega\Phi(x)$ is equivalent to the Dirac system of two first-order ODE's:

$$-i\frac{d\phi_2}{dx} = (\omega + m)\phi_1(x), \tag{30}$$
$$-i\frac{d\phi_1}{dx} = (\omega - m)\phi_2(x). \tag{31}$$

The solution of the system (30)–(31) is identical to the solution of the previous system but the "electrostatic"matching conditions must be conjugated:

$$\begin{pmatrix}\phi_1(0^+)\\ \phi_2(0^+)\end{pmatrix} = \begin{pmatrix}\cos q & i\sin q\\ i\sin q & \cos q\end{pmatrix}\begin{pmatrix}\phi_1(0^-)\\ \phi_2(0^-)\end{pmatrix}. \tag{32}$$

Our goal is to search for, bound states, i.e., $|\omega| < |m|$, and scattering states, i.e., $|\omega| > |m|$, both for the case of electrons and positrons.

3.1. Relativistic Electron and Positron Bound States

In order to compute bound states, exponentially decaying solutions of (27)–(28) system in zone I must be related to exponentially decaying solutions of the same system in zone II by implementing the electrostatic matching conditions (29) to identify the electron bound states and identical procedure will provide positron bound states replacing the ODE system by (30)–(31) and using the matching condition (32).

- **Zone I**: $x < 0$

$$\psi_1^I(x,\kappa) = A^I(\kappa)e^{\kappa x}, \quad \psi_2^I(x,\kappa) = B^I(\kappa)e^{\kappa x}, \quad \kappa > 0.$$

Plugging this ansatz in the spectral equation system (27)–(28) one finds a linear algebraic homogeneous system in A^I and B^I whose solution (taking into account that the value of the energy $\omega = \sqrt{m^2 - \kappa^2}$ is compatible with bound states in zone I provided that $0 < \kappa < |m|$) is the following eigenspinor:

$$\Psi_+^I(x,\kappa) = A_+^I(\kappa)\begin{pmatrix}1\\ \frac{-i\kappa}{\omega+m}\end{pmatrix}e^{\kappa x}. \tag{33}$$

- **Zone II**: $x > 0$

$$\psi_1^{II}(x,\kappa) = A^{II}(\kappa)e^{-\kappa x}, \quad \psi_2^{II}(x,\kappa) = B^{II}(\kappa)e^{-\kappa x}, \quad \kappa > 0.$$

Similarly, plugging this ansatz in the spectral equation system (27)–(28) one finds a linear algebraic homogeneous system in A^{II} and B^{II} whose solution (taking into account the possible value of the energy ω compatible with the existence of bound states in zone II provided that $0 < \kappa < |m|$) is the following eigenspinor:

$$\Psi_+^{II}(x,\kappa) = A_+^{II}(\kappa)\begin{pmatrix}1\\ \frac{i\kappa}{\omega+m}\end{pmatrix}e^{-\kappa x}. \tag{34}$$

In order to join the eigenspinors in zone I with those in zone II at $x = 0$, we impose the matching conditions at the origin (29) and obtain the linear homogeneous system:

$$\begin{pmatrix}-\cos q + \frac{\kappa\sin q}{\omega+m} & 1\\ i(\sin q + \frac{\kappa\cos q}{\omega+m}) & \frac{i\kappa}{\omega+m}\end{pmatrix}\cdot\begin{pmatrix}A_+^I\\ A_+^{II}\end{pmatrix} = \begin{pmatrix}0\\ 0\end{pmatrix}. \tag{35}$$

Non null solutions of the homogeneous system (35) correspond to the roots of the determinant of the previous 2×2 matrix. In the same way, imposing similar anstaz for the ϕ field and solving the spectral equation system (30)–(31) the possible eigenstates take the form

- **Zone I**: $x < 0$

$$\Phi_+^I(x,\kappa) = D_+^I(\kappa)\begin{pmatrix}\frac{-i\kappa}{\omega+m}\\ 1\end{pmatrix}e^{\kappa x}. \tag{36}$$

- **Zone II**: $x > 0$

$$\Phi_+^{II}(x,\kappa) = D_+^{II}(\kappa)\begin{pmatrix}\frac{i\kappa}{\omega+m}\\ 1\end{pmatrix}e^{-\kappa x}. \tag{37}$$

Relating the spinors in both zones through the matching condition for positrons in $x = 0$ (32) we obtain the linear homogeneous system

$$\begin{pmatrix}-\cos q - \frac{\kappa\sin q}{\omega+m} & 1\\ i(-\sin q + \frac{\kappa\cos q}{\omega+m}) & \frac{i\kappa}{\omega+m}\end{pmatrix}\cdot\begin{pmatrix}D_+^I\\ D_+^{II}\end{pmatrix} = \begin{pmatrix}0\\ 0\end{pmatrix}, \tag{38}$$

that allow us to obtain the bound states of positrons.

Since the parameter q is an angle and because the δ-potential is defined by means of trigonometric functions, the signs of κ, ω change in every quadrant. The outcome is that there exists one

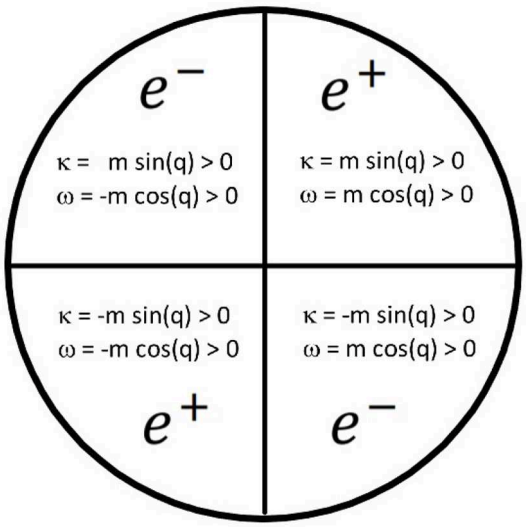

FIGURE 1 | Bound states for electrons and positrons in an electrostatic δ-potential ($\lambda = 0$).

bound state in each quadrant, two for electrons and two for positrons, distributed as shown in the **Figure 1**.

These bound states correspond to one positive energy electron trapped in either one positive or negative energy state and one positive energy positron trapped alternatively in positive or negative energy states. This structure is periodic in q.

Positron bound states

1. $0 < q < \frac{\pi}{2}; \kappa_b = m \sin q > 0, \omega_b = \sqrt{m^2 - \kappa_b^2} = m \cos q > 0$

$$D_+^{II} = D_+^I,$$
$$\Phi(x, \kappa_b) = D_+ \begin{pmatrix} i\,\mathrm{sign}(x)\frac{\sin q}{1+\cos q} \\ 1 \end{pmatrix} e^{-m|x|\sin q}. \quad (39)$$

2. $\pi < q < \frac{3\pi}{2}; \kappa_b = -m \sin q > 0, \omega_b = \sqrt{m^2 - \kappa_b^2} = -m \cos q > 0$

$$D_+^{II} = -D_+^I,$$
$$\Phi(x, \kappa_b) = D_+ \begin{pmatrix} \frac{i \sin q}{1-\cos q} \\ -\mathrm{sign}(x) \end{pmatrix} e^{m|x|\sin q}. \quad (40)$$

Electron bound states

1. $\frac{\pi}{2} < q < \pi; \kappa_b = m \sin q > 0, \omega_b = \sqrt{m^2 - \kappa_b^2} = -m \cos q > 0$

$$A_+^{II} = -A_+^I,$$
$$\Psi(x, \kappa_b) = A_+ \begin{pmatrix} -\mathrm{sign}(x) \\ \frac{-i \sin q}{1-\cos q} \end{pmatrix} e^{-m|x|\sin q}. \quad (41)$$

2. $\frac{3\pi}{2} < q < 2\pi; \kappa_b = -m \sin q > 0, \omega_b = \sqrt{m^2 - \kappa_b^2} = m \cos q > 0$

$$A_+^{II} = A_+^I,$$
$$\Psi(x, \kappa_b) = A_+ \begin{pmatrix} 1 \\ -i\,\mathrm{sign}(x)\frac{\sin q}{1+\cos q} \end{pmatrix} e^{m|x|\sin q}. \quad (42)$$

It is worthwhile to mention that if $q = \frac{\pi}{2}$ or $q = \frac{3\pi}{2}$ zero modes exist. For instance when $q = \frac{\pi}{2}$ we have $\kappa_b = m, \omega_b = 0$ whereas the eigenspinor reads:

$$\Phi(x, m) = D_+ \begin{pmatrix} i\,\mathrm{sign}(x) \\ 1 \end{pmatrix} e^{-m|x|}.$$

We stress that the bound states just described are closer to the bound states in the scalar case with mixed potential of the form $V(x) = -a\delta(x) + b\delta'(x)$ (see [23]). In both cases the normalizable wave functions exhibit finite discontinuities at the origin.

3.2. On the Charge Density

The charge density can be written as:

$$j^0(t,x) = \pm Q\,\overline{\varphi}(t,x)\gamma^0\varphi(t,x) = \pm Q\,\varphi^\dagger(t,x)\varphi(t,x)$$
$$= \pm Q\,\left(\varphi_1^*(t,x)\varphi_1(t,x) + \varphi_2^*(t,x)\varphi_2(t,x)\right), \quad (43)$$

being Q a positive constant and taken into account that $+$ will be chosen in the case of electrons and $-$ for positrons. On the one hand, if we substitute the positron bound states (39, 40) in (43) the charge density obtained is

$$j_0(x) = -m\,Q\,\sin q\, e^{-2m|x|\sin q}, \quad \text{iff} \quad 0 < q < \frac{\pi}{2}. \quad (44)$$
$$j_0(x) = +m\,Q\,\sin q\, e^{2m|x|\sin q}, \quad \text{iff} \quad \pi < q < \frac{3\pi}{2}. \quad (45)$$

On the other hand, if we substitute the electron bound states (41, 42) in (43) the charge density obtained is

$$j_0(x) = +m\,Q\,\sin q\, e^{-2m|x|\sin q}, \quad \text{iff} \quad \frac{\pi}{2} < q < \pi. \quad (46)$$
$$j_0(x) = -m\,Q\,\sin q\, e^{2m|x|\sin q}, \quad \text{iff} \quad \frac{3\pi}{2} < q < 2\pi. \quad (47)$$

All the results are shown in **Figure 2**.

3.3. Relativistic Electron and Positron Scattering Spinors

We pass to study the scattering of 1D Dirac particles through a Dirac electrostatic δ-potential ($V(x) = q\delta(x)\mathbb{1}$) in order to obtain the scattering amplitudes. On the one hand, electron scattering spinors coming from the left toward the δ-impurity ("diestro"scattering) have the form:

$$\Psi^R(x,k) = \begin{cases} u_+(k)\,e^{ikx} + \rho_R(k)\,\gamma^0 u_+(k)\,e^{-ikx}, & x < 0 \\ \sigma_R(k)\,u_+(k)\,e^{ikx}, & x > 0 \end{cases}, \quad (48)$$

where $u_+(k)$ is the positive energy electron spinor that solves the free static Dirac equation for plane waves moving along the real line (23). The solutions in both zones are related at the origin through the electrostatic δ-matching conditions (10) if and only if the transmission and reflection scattering amplitudes are:

$$\sigma_R(k) = \frac{k}{k\cos q + i\sqrt{k^2+m^2}\,\sin q},$$

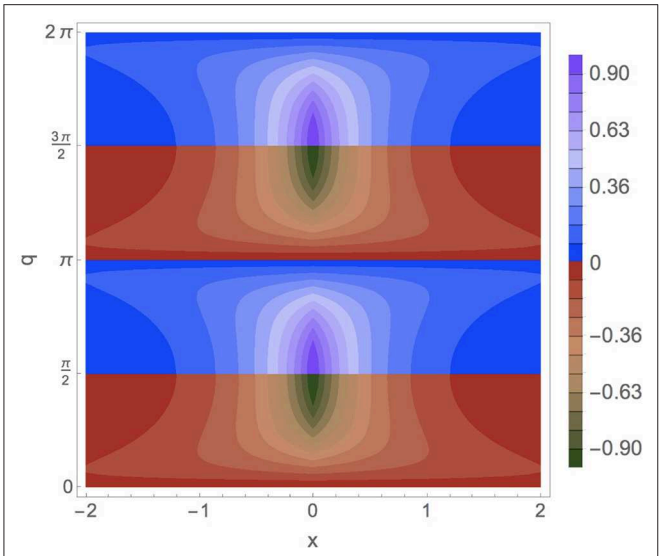

FIGURE 2 | Charge density as a function of x when $Q = m = 1$ and $\lambda = 0$ (electrostatic δ-potential). For $0 < q < \pi/2$ and $\pi < q < 3\pi/2$ the charge densities of a positron bound state are plotted [(44), (45), respectively]. For $\pi/2 < q < \pi$ and $3\pi/2 < q < 2\pi$ the charge densities of a electron bound state are plotted [(46), (47), respectively].

$$\rho_R(k) = -\frac{i\, m \sin q}{k\cos q + i\sqrt{k^2+m^2}\sin q}, \tag{49}$$

which obviously satisfy the unitarity condition: $\left|\sigma_R(k)\right|^2 + \left|\rho_R(k)\right|^2 = 1$. On the other hand, electrons coming from the right toward the δ-impurity, ("zurdo"scattering), are described by spinors of the form

$$\Psi^L(x,k) = \begin{cases} \sigma_L(k)\,\gamma^0 u_+(k)\, e^{-ikx}, & x<0 \\ \rho_L(k)\, u_+(k)\, e^{ikx} + \gamma^0 u_+(k)\, e^{-ikx}, & x>0 \end{cases}, \tag{50}$$

The δ-well matching conditions (10) for this "zurdo" scattering ansatz are satisfied if $\sigma_R(k) = \sigma_L(k)$ and $\rho_R(k) = \rho_L(k)$. It is worth noting that

- Since the scattering amplitudes for "diestro"and "zurdo"scattering of the electrons through an electrostatic δ-potential are identical, the processes governed by this potential are parity and time-reversal invariants.
- Purely imaginary poles $k = i\kappa$ of the transmission amplitude σ are the bound states of the spectrum if κ is real and positive. In formula (49) we observe that poles of this type appear if the imaginary momentum satisfies the equation

$$\frac{\kappa_b}{\sqrt{m^2-\kappa_b^2}} = -\tan q,$$

which admits positive solutions for κ_b only if $\tan q < 0$, i.e., if q lives in the second or fourth quadrant. Moreover, explicit solutions of the previous equation are: $\kappa_b = \pm m \sin q$, i.e., assuming that $m > 0$ the plus sign must be selected in the second quadrant and the minus sign is valid in the fourth quadrant.

- Probability is conserved even in this relativistic quantum mechanical context provided that $\omega^2 > m^2$, $m > 0$.

For positrons, the "diestro"scattering ansatz of the spinor (that is a solution of the conjugate Dirac equation in zones I and II) is

$$\Phi^R(x,k) = \begin{cases} v_+(k)\, e^{-ikx} - \tilde{\rho}_R(k)\,\gamma^0 v_+(k)\, e^{ikx}, & x<0 \\ \tilde{\sigma}_R(k)\, v_+(k)\, e^{-ikx}, & x>0 \end{cases}, \tag{51}$$

where $v_+(k)$ is the positive energy positron spinor that represents plane waves moving along the real line (25). By imposing the matching conditions on $x = 0$ (18), the following scattering coefficients are obtained

$$\begin{aligned} \tilde{\sigma}_R(k) &= \frac{k}{k\cos q - i\sqrt{k^2+m^2}\sin q}, \\ \tilde{\rho}_R(k) &= \frac{i\, m \sin q}{k\cos q - i\sqrt{k^2+m^2}\sin q}. \end{aligned} \tag{52}$$

Again, unitarity is preserved: $\left|\tilde{\sigma}(k)\right|^2 + \left|\tilde{\rho}_R(k)\right|^2 = 1$.

The "zurdo"positron scattering ansatz, however, takes the form

$$\Phi^L(x,k) = \begin{cases} -\tilde{\sigma}_L(k)\,\gamma^0 v_+(k)\, e^{ikx}, & x<0 \\ \tilde{\rho}_L(k)\, v_+(k)\, e^{-ikx} - \gamma^0 v_+(k)\, e^{ikx}, & x>0 \end{cases}, \tag{53}$$

Again, by imposing the matching conditions on $x = 0$ (18), we find that $\tilde{\sigma}_L(k) = \tilde{\sigma}_R(k)$ and $\tilde{\rho}_L(k) = \tilde{\rho}_R(k)$. It is worth noting that

- The scattering amplitudes for "diestro" and "zurdo" scattering of positrons through an electrostatic δ-well are identical: there is no violation of parity and time reversal invariance in the scattering of positrons by δ-impurities.
- The purely imaginary $k = i\kappa$ poles of $\tilde{\sigma}$ are the positron bound states in the spectrum of the conjugate Dirac Hamiltonian. In formula (52) we observe that poles of this type appear if the imaginary momentum satisfies the equation

$$\frac{\kappa_b}{\sqrt{m^2-\kappa_b^2}} = \tan q,$$

which admits positive solutions for κ_b only if $\tan q > 0$, i.e., if q lives in the first or third quadrant. Between the explicit solutions of this equation, $\kappa_b = \pm m \sin q$, the plus sign must be chosen in the first quadrant, and the minus sign in the third quadrant assuming that $m > 0$.

- The relations between diestro and zurdo scattering amplitudes for electrons and positrons are as follows:

$$\begin{aligned} \sigma_R(k) = \sigma_L(k) = \tilde{\sigma}_R^*(k) = \tilde{\sigma}_L^*(k), \\ \rho_R(k) = \rho_L(k) = \tilde{\rho}_R^*(k) = \tilde{\rho}_L^*(k). \end{aligned} \tag{54}$$

The unitary $\boldsymbol{S}$-matrix

$$\boldsymbol{S} = \begin{pmatrix} \sigma(k) & \rho(k) \\ \rho(k) & \sigma(k) \end{pmatrix} \quad , \quad \boldsymbol{S}^{\dagger} \cdot \boldsymbol{S} = \boldsymbol{I},$$

encodes the phase shifts in its spectrum; $\lambda_{\pm} = \sigma \pm \rho = e^{2i\delta_{\pm}(k)}$. The phase shifts $\delta_{\pm}(k)$ in the even and odd channels are thus

$$\tan 2\delta_{\pm}(k) = \frac{\mathrm{Im}(\sigma(k) \pm \rho(k))}{\mathrm{Re}(\sigma(k) \pm \rho(k))},$$

whereas the total phase shift $\delta(k) = \delta_{+}(k) + \delta_{-}(k)$ is easily derived:

$$\tan 2\delta(k) = \frac{\mathrm{Im}[\sigma^2(k) - \rho^2(k)]}{\mathrm{Re}[\sigma^2(k) - \rho^2(k)]} = \frac{2k\sqrt{k^2+m^2}\sin(2q)}{m^2 - (2k^2+m^2)\cos(2q)}.$$

4. "MASS-SPIKE"δ-POTENTIAL

Next, we consider the one-dimensional Dirac Hamiltonian with a single Dirac δ-potential disturbing the mass term:

$$H_{\mathrm{M}\delta} = -i\sigma_1 \frac{d}{dx} + (m + \lambda\delta(x))\sigma_3.$$

4.1. Relativistic Bound States in Mass-Spike δ Wells

Firstly, we will search for bound states where electrons and positrons are trapped by mass-spike δ wells. In the case of electrons, away from the singularity the positive energy spinors take the form (33, 34). The continuation to the whole real line is achieved by applying to those spinors the relativistic matching conditions at the origin $x = 0$ (12) as follows:

$$\begin{pmatrix} \psi^{II}_{1+}(0,\kappa) \\ \psi^{II}_{2+}(0,\kappa) \end{pmatrix} = \begin{pmatrix} \cosh\lambda & i\sinh\lambda \\ -i\sinh\lambda & \cosh\lambda \end{pmatrix} \begin{pmatrix} \psi^{I}_{1+}(0,\kappa) \\ \psi^{I}_{2+}(0,\kappa) \end{pmatrix} \quad (55)$$

In this way, we obtain the following homogeneous algebraic system written in matrix form as:

$$\begin{pmatrix} -\left(\cosh\lambda + \frac{\kappa\sinh\lambda}{m+\sqrt{m^2-\kappa^2}}\right) & 1 \\ i\left(\frac{\kappa\cosh\lambda}{m+\sqrt{m^2-\kappa^2}} + \sinh\lambda\right) & \frac{i\kappa}{m+\sqrt{m^2-\kappa^2}} \end{pmatrix} \begin{pmatrix} A^{I}_{+} \\ A^{II}_{+} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \quad (56)$$

The determinant of this 2×2 matrix is zero such that there is a non null solution of (56) if $\kappa_b = -m\tanh\lambda$ which provides a normalizable spinor only if $\lambda < 0$. The energy of the electron bound state is $\omega_b = m\,\mathrm{sech}\lambda$. This bound state spinor is extended to the whole line by means of the condition $A^{II}_{+} = A^{I}_{+}$, i.e., the spinor takes the form:

$$\Psi_{+}(x,\kappa_b) = A_{+}\begin{pmatrix} 1 \\ -i\,\mathrm{sign}(x)\frac{\sinh\lambda}{1+\cosh\lambda} \end{pmatrix} e^{m|x|\tanh\lambda}. \quad (57)$$

The charge density of this bound state is obtained by replacing the spinor (57) in the equation (43), arriving at the result

$$j_0(x) = -m\,Q\tanh\lambda\, e^{2m|x|\tanh\lambda}, \quad (58)$$

which is represented in **Figure 3**.

Investigation of positron bound states requires applying the same relativistic matching conditions (12) at the origin to the bound state positron spinors (36)–(37) in order to obtain the following homogeneous algebraic system written in matrix form as:

$$\begin{pmatrix} i\left(\frac{\kappa\cosh\lambda}{m+\sqrt{m^2-\kappa^2}} - \sinh\lambda\right) & \frac{i\kappa}{m+\sqrt{m^2-\kappa^2}} \\ -\cosh\lambda + \frac{\kappa\sinh\lambda}{m+\sqrt{m^2-\kappa^2}} & 1 \end{pmatrix} \begin{pmatrix} D^{I}_{+} \\ D^{II}_{+} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \quad (59)$$

The determinant of this 2×2 matrix is zero such that there is a non null solution of (59) if $\kappa_b = m\tanh\lambda$. This imaginary momentum provides a normalizable spinor only if $\lambda > 0$. The energy of this positron bound state is $\omega_b = m\,\mathrm{sech}\lambda$. The spinor bound state is extended to the whole line by means of the condition $D^{II}_{+} = D^{I}_{+}$:

$$\Phi_{+}(x,\kappa_b) = D_{+}\begin{pmatrix} i\,\mathrm{sign}(x)\frac{\sinh\lambda}{1+\cosh\lambda} \\ 1 \end{pmatrix} e^{-m|x|\tanh\lambda}. \quad (60)$$

The charge density of this bound state is obtained by replacing the spinor (60) in the equation (43), arriving at the result

$$j_0(x) = -m\,Q\tanh\lambda\, e^{-2m|x|\tanh\lambda}, \quad (61)$$

which is represented in **Figure 4**.

4.2. Electron and Positron Scattering Spinors

To obtain the scattering amplitudes for electrons coming from the left ("diestro"scattering) on mass-spike impurities the free spinors in zones I and II away from the origin (48) must be joined by using the $\mathbb{SU}(1,1)$ matrix appearing in (55). More explicitly,

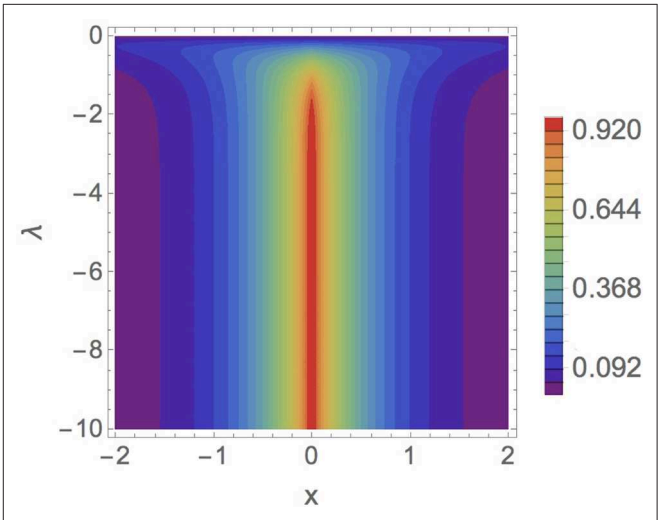

FIGURE 3 | Charge density (58) as a function of x for electrons when $Q = m = 1$ and $q = 0$ (mass-spik δ-potential).

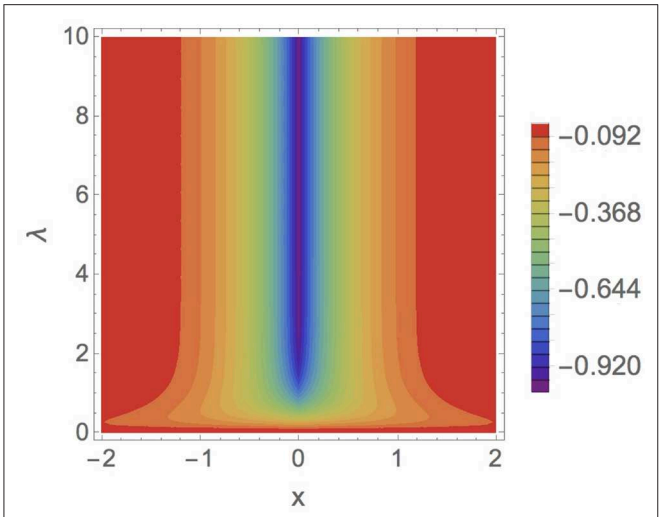

FIGURE 4 | Charge density (61) as a function of x for positrons when $Q = m = 1$ and $q = 0$ (mass-spike δ-potential).

this matching sets an algebraic system whose solutions are the scattering coefficients:

$$\sigma_R(k) = \frac{k}{k\cosh\lambda + im\sinh\lambda}\,, \quad \rho_R(k) = \frac{-i\sqrt{k^2+m^2}\sinh\lambda}{k\cosh\lambda + im\sinh\lambda},$$

which obviously respect probability conservation:

$$\left|\sigma_R(k)\right|^2 + \left|\rho_R(k)\right|^2 = 1.$$

Repeating this procedure for the "zurdo"scattering spinorial ansatz (50) we conclude with the same relativistic δ-interaction scattering amplitudes as in "diestro"scattering. In sum

- The scattering amplitudes for diestro and zurdo scattering of electrons through a mass-spike δ-interaction are identical. This means that the mass-spike δ interaction respect both parity and time-reversal symmetries.
- The $\boldsymbol{S}$-matrix is unitary and the phase shifts appear as the exponents of its eigenvalues. The total phase shift is:

$$\tanh 2\delta(k) = \frac{\mathrm{Im}[\sigma^2(k)-\rho^2(k)]}{\mathrm{Re}[\sigma^2(k)-\rho^2(k)]} = \frac{-2km\sinh 2\lambda}{k^2+m^2+(k^2-m^2)\cosh 2\lambda}\,.$$

- The purely imaginary poles of the transmission amplitude $\sigma(k)$ with positive imaginary part are the bound states of the spectrum and occur when: $k_b = i\kappa_b = -im\tanh\lambda$, i.e., $\omega_b = m\,\mathrm{sech}\lambda$. It must be fulfilled that $\tanh\lambda < 0$.

Investigation of the positron "diestro"scattering amplitudes is achieved by imposing the relativistic matching conditions

$$\Phi^{II}_{+}(0,k) = \begin{pmatrix} \cosh\lambda & i\sinh\lambda \\ -i\sinh\lambda & \cosh\lambda \end{pmatrix} \cdot \Phi^{I}_{+}(0,k),$$

on the positron spinor scattering ansatz (51). This criterion is tantamount to an algebraic system for the scattering amplitudes whose solutions are:

$$\tilde{\sigma}_R(k) = \frac{k}{k\cosh\lambda - im\sinh\lambda}\,, \quad \tilde{\rho}_R(k) = \frac{i\sqrt{k^2+m^2}\sinh\lambda}{k\cosh\lambda - im\sinh\lambda},$$

which also respects probability conservation:

$$\left|\tilde{\sigma}_R(k)\right|^2 + \left|\tilde{\rho}_R(k)\right|^2 = 1\,.$$

To avoid repetitions, we skip a detailed computing of the positron scattering amplitudes for "zurdo"scattering, we merely states that are identical to the scattering amplitudes for positrons coming from the left toward the δ-obstacle. Thus, we summarize the main features of positron scattering through a mass-spike δ-imputity as follows:

- The scattering amplitudes for diestro and zurdo scattering of positrons through a mass-spike δ-interaction are identical to each other. Therefore, there is no breaking of either parity or time-reversal symmetries.
- The $\boldsymbol{S}$-matrix is unitary and the phase shifts appears as the exponents of its eigenvalues. The total phase shifts for positrons are

$$\tanh 2\tilde{\delta}(k) = \frac{\mathrm{Im}[\tilde{\sigma}^2(k)-\tilde{\rho}^2(k)]}{\mathrm{Re}[\tilde{\sigma}^2(k)-\tilde{\rho}^2(k)]} = \frac{2km\sinh 2\lambda}{k^2+m^2+(k^2-m^2)\cosh 2\lambda}\,.$$

- The purely imaginary poles of the transmission amplitude $\tilde{\sigma}(k)$ with positive imaginary part are the positron bound states of the spectrum and occur when $k_b = i\kappa_b = im\tanh\lambda$, i.e., $\omega_b = m\,\mathrm{sech}\lambda$. It must be fulfilled that $\tanh\lambda > 0$.
- The relations between diestro and zurdo scattering amplitudes for electrons and positrons in a mass-spike δ-potential are as follows:

$$\begin{aligned} &\sigma_R(k) = \sigma_L(k) = \tilde{\sigma}^*_R(k) = \tilde{\sigma}^*_L(k), \\ &\rho_R(k) = \rho_L(k) = \tilde{\rho}^*_R(k) = \tilde{\rho}^*_L(k). \end{aligned} \tag{62}$$

5. SUMMARY AND OUTLOOK

The spectrum of the 1D Dirac Hamiltonian providing the one-particle spectrum for 1D electrons and positrons has been analyzed when there is one impurity that distorts the free propagation of fermions. We have implemented the impurity by means of Dirac δ-potentials of two types that we denote respectively as electrostatic and mass-spike according to their physical meaning.

In the electrostatic case (where the coupling is an angle) we find that:

1. There are two quadrants ($\pi/2 < q < \pi$ and $3\pi/2 < q < 2\pi$) where the coupling of the δ-interaction gives rise to one electron bound state. One positron bound state arise in the other two quadrants ($0 < q < \pi/2$ and $\pi < q < 3\pi/2$).

2. Regarding scattering amplitudes we found that positrons and electrons are scattered by the impurity so that the electron scattering coefficients are the conjugate of the positron ones.

For mass-spike δ-potentials our results are:

1. There is one bound state of electrons if the coupling is negative and other one of positrons if the coupling is positive.
2. The scattering amplitudes of electrons due to a mass-spike δ-impurity are the conjugate of positrons ones.

We plan to continue this investigation along the following lines of research:

- First, our purpose is to study the effect on free fermions of an impurity carrying both electrostatic and mass-spike couplings.
- Second, it is our intention to consider two, several or even infinity δ-impurities (often called as δ-comb potential), as the periodic potentials arise in various materials models.
- Third, after having managed all these tasks, we envisage to compute quantum vacuum energies and Casimir forces induced by these 1D fermions, in a parallel analysis to that performed for bosons in [17] and references quoted therein.

DATA AVAILABILITY

The raw data supporting the conclusions of this manuscript will be made available by the authors, without undue reservation, to any qualified researcher.

AUTHOR CONTRIBUTIONS

All authors listed have made a substantial, direct and intellectual contribution to the work, and approved it for publication.

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Point-Particle Catalysis

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We use the point-particle effective field theory (PPEFT) framework to describe particle-conversion mediated by a flavor-changing coupling to a point-particle. We do this for a toy model of two non-relativistic scalars coupled to the same point-particle, on which there is a flavor-violating coupling. It is found that the point-particle couplings all must be renormalized with respect to a radial cut-off near the origin, and it is an invariant of the flow of the flavor-changing coupling that is directly related to particle-changing cross-sections. At the same time, we find an interesting dependence of those cross-sections on the ratio $k_{\rm out}/k_{\rm in}$ of the outgoing and incoming momenta, which can lead to a $1/k_{\rm in}$ enhancement in certain regimes. We further connect this model to the case of a single-particle non-self-adjoint (absorptive) PPEFT, as well as to a PPEFT of a single particle coupled to a two-state nucleus. These results could be relevant for future calculations of any more complicated reactions, such as nucleus-induced electron-muon conversions, monopole catalysis of baryon number violation, as well as nuclear transfer reactions.

Keywords: flavor violation, effective field theories, catalysis, high energy physics - theory, nuclear theory

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1. INTRODUCTION

It is often the case that physically interesting situations involve a hierarchy of characteristic scales. For instance, solar system dynamics involve a variety of length scales, such as the sizes of the stars and planets involved, as well as the sizes of the orbits. Exploiting such a hierarchy by means of judicious Taylor expansions can greatly simplify otherwise very difficult problems, frequently even providing a handle on seemingly intractable problems. In the realm of quantum field theory, this insight has led to the development of the highly successful effective field theories, which can reduce the complexity of quantum field theories by restricting to parameter subspaces in which an appropriate Taylor expansion can be used to put the theory into a simpler form.

Usually, effective field theories exploit the hierarchy between interaction energies and the masses of some heavy particles to remove those heavy particles from the theory altogether (the quintessential example being Fermi's theory of the Weak interaction, which removes the heavy W and Z bosons) [1–4]. However, it is often the case that one's interest lies in a sector of the theory that still contains one or two of the heavy particles. For instance, in an atom, a heavy nucleus is present, but for most purposes there is no need to go about computing loops of nucleus-anti-nucleus pairs. Instead, higher energy nuclear dynamics are seen as finite nuclear-size effects. For this reason, an EFT has recently been explored that describes the remnant heavy particles in position-space to exploit the hierarchy of energy scales in a more intuitive expansion in kR, where k is the (small) momentum of the light particle and R is the length-scale of the nuclear structure [5–7]. This is accomplished in a simple way; the usual effective action is supplemented by a "point-particle" action that involves all possible couplings of the light particle to the worldline of the remnant heavy (point-like) particle (consistent with the symmetries of the low-energy theory). This type of "point-particle" EFT (PPEFT) is conceptually the next best thing to a Fermi type of EFT. While the nuclear

dynamics cannot be removed altogether, they are significantly simplified.

The practicality of a PPEFT is two-fold: first it easily permits parameterizing physical quantities in terms of small nuclear properties, since the PPEFT expansion is directly in powers of kR. Second, that parameterization is completely general, and inherently includes all possible interactions, including any potential new physics. Some obvious examples that have been explored are cross-sections and bound-state energies of electrons in terms of nuclear charge radii [7, 8]. In this work, we ask the question: how do the small nuclear properties enter into physical quantities when there are multiple channels of interaction with the point-particle? (We ask this with mind toward eventually describing nuclear transfer reactions, and possibly baryon-monopole reactions which are known to suffer from questions of self-adjointedness of the Hamiltonian similar to those we address in this article [9, 10]).

To answer this question, we consider a simple toy model of two bulk Schrödinger (complex) fields coupled to the same point particle. The most general couplings to the point-particle's worldline $y^\mu(\tau)$ are easily generalized from the single particle species (SP) examples explored in Burgess et al. [5] to the multi-particle (MP) case.

$$\begin{aligned} S_b^{(\mathrm{SP})} &= -\int d\tau \sqrt{-\dot{y}^2}\,[M + h\,\Psi^*\Psi + \dots] \quad \longrightarrow \\ S_b^{(\mathrm{MP})} &= -\int d\tau \sqrt{-\dot{y}^2}\,[M + \Psi_i^* h_{ij} \Psi_j + \dots], \end{aligned} \tag{1.1}$$

where Ψ, Ψ_i are bulk (complex) scalars, and the flavor index runs over 1 and 2. h_{ij} is a matrix of coupling constants that generalizes the single-particle coupling h, and the integral is over the proper time τ of the point-particle ($\dot{y}^\mu := \frac{dy^\mu}{d\tau}$ is the point-particle's 4-velocity). Away from the point-particle, the action is just the usual Schrödinger action for (now) two scalars,

$$\begin{aligned} S_B^{(\mathrm{MP})} = \sum_{i=1}^{2} \int d^4x \, \Big\{ & \frac{i}{2}\left(\Psi_i^* \partial_t \Psi_i - \Psi_i \partial_t \Psi_i^*\right) \\ & - \frac{1}{2m_i} |\nabla \Psi_i|^2 - V(r) |\Psi_i|^2 \Big\}. \end{aligned} \tag{1.2}$$

[$V(r)$ is some bulk potential that may be sourced by the point-particle. In the main text we take it to be an inverse-square potential, since such a potential is highly singular and known to drive interesting behavior in a PPEFT [5]. For the moment it suffices to drop the potential]. If the bulk action (1.2) diagonalizes the momentum it need not diagonalize the brane action (1.1), and it is possible the off-diagonal elements of $\mathbf{h}$ (the matrix of h_{ij}) can source flavor-violating interactions.

In the center-of-mass reference frame (in the limit of infinite point-particle mass[1]), the action (1.1) acts as a boundary condition at the origin for the modes of the Ψ_i fields. However, in general those diverge, and so the action has to be regulated at some finite radius ϵ. The couplings $\mathbf{h}$ must then be renormalized to keep physical quantities independent of the regulator, and it turns out that the (low-energy s-wave) cross-section for flavor violation is directly related to an invariant (ϵ_3) of the RG-flow of the off-diagonal h_{12}:

$$\sigma_s^{(1\to 2)} = 4\pi \frac{k_2}{k_1} \epsilon_3^2, \tag{1.3}$$

where k_1 and k_2 are the incoming and outgoing momenta, respectively. For Schrödinger particles, the factor $k_2/k_1 = \sqrt{m_2/m_1}$ is a constant. However, the same formula holds for spinless relativistic particles, and the ratio $k_2/k_1 = \sqrt{(k_1^2 + m_1^2 - m_2^2)/k_1^2}$ leads to different qualitative behaviors of the low-energy cross-section depending on how k_1 relates to the mass gap $m_1^2 - m_2^2$. If the mass gap is positive, and $k_1^2 \ll m_1^2 - m_2^2$, then the cross-section exhibits a $1/k_1$ enhancement. Both the dependence on ϵ_3 and on k_1 may prove to be useful in a more complicated calculation, such as in mesic transfer reactions $\pi^0 + p \to \pi^+ + n$ (where the neutron and proton are in a nucleus), or possible flavor changing reactions involving new physics, such as $\mu^- + N \to e^- + N$ [11, 12].

The channels of interaction with the point-particle do not have to be different bulk species, however. If, for example, the nucleus carried two accessible energy states, say $E_\uparrow = M + \Delta/2$ and $E_\downarrow = M - \Delta/2$ (where $\Delta \ll M$ is some small excitation energy), then two channels of interaction could be a single bulk particle interacting with each of the nuclear energy eigenstates. In this case the "flavor-violating" cross section is again (1.3), where now k_1 and k_2 are the incoming and outgoing single-particle momenta, and $k_2/k_1 = k_{\mathrm{out}}/k_{\mathrm{in}} = \sqrt{(k_{\mathrm{in}}^2 \pm 2m\Delta)/k_{\mathrm{in}}^2}$ with the $\pm$ corresponding to the bulk particle impinging on a nucleus in the ground state ($-$) or the excited state ($+$), and where m is the mass of the single bulk species (recall we work in the non-recoil limit). On its own, this description is enough for any simple reaction $\psi + N \to \psi + N^*$, where an incident non-relativistic particle just knocks a nucleus into a long-lived slightly energized state. Together, the two-species and two-nuclear state models form the building blocks for exploring more complicated processes, such as nuclear transfer reaction, where an incident particle exchanges some constituent particles with a nucleus, and the final state *both* violates flavor of the bulk species *and* changes the state of the source nucleus.

Finally, we can also look toward simpler models instead. One may imagine for instance only being interested in tracking one of the bulk-species, say particle 1 (perhaps an apparatus can only detect particles of flavor 1). In that case, the flavor-violating cross-section appears as an absorptive interaction when restricting to the particle 1 subspace of the theory. In this way, our toy model can be seen as a particular unitary completion of a model with a single particle subject to a non-self-adjoint Hamiltonian, as studied in Plestid et al. [13] and frequently used in the form of nuclear optical models [14, 15].

The rest of this paper is organized as follows. First, we briefly recall the salient details of a simple PPEFT for a single bulk species. Then in section 3, we establish the action and

[1]We neglect here recoil effects, though those can be included by tracking the dynamics of $y^\mu(\tau)$.

classical solutions to a point-particle EFT involving two bulk species, followed by section 4 in which we solve the boundary conditions of the system, and determine how all of the point-particle couplings run. All of this comes together in section 5 where we compute how the point-particle properties relate to physical cross-sections, including the cross-section for flavor-violation. In section 6 we connect the multi-bulk species story to a single particle coupled to a two-state nucleus. Finally, we wrap up in section 7 by restricting to a single-particle subsector of the multi-species model, and realizing the equivalence to the absorptive model of Plestid et al. [13].

2. POINT-PARTICLE EFT FOR A SINGLE BULK SPECIES

We review the point-particle effective field theory for a single Schrödinger particle in an inverse-square potential, first described in Burgess et al. [5].

In the point-particle effective field theory approach, we exploit the hierarchy of length-scales between the characteristic wavelength of some low-energy particle of mass m (for concreteness, call this some scalar electron) and the scale of some small, almost point-like particle of mass $M \gg m$ it interacts with (similarly, we will call this a nucleus). For example, in atomic systems, this would be the ratio R/a_0 between the size R of a nucleus and the Bohr radius a_0 of the atom. For scattering, the small parameter is more directly kR, with k the wavenumber of the incident particle. The way we exploit this hierarchy is to recall that the low energy dynamics of the heavy particle are well approximated by ordinary quantum mechanics, so we imagine only first-quantizing the nucleus. In that case the fully second-quantized electron only couples to the 1-dimensional world-line of the heavy particle. This amounts to writing the action for the electron $S = S_B + S_b$ in terms of the usual bulk dynamics[2]

$$S_B = \int d^4x \left\{ \frac{i}{2}\left(\Psi^*\partial_t\Psi - \Psi\,\partial_t\Psi^*\right) - \frac{1}{2m}|\nabla\Psi|^2 - V(r)|\Psi|^2 \right\} \tag{2.1}$$

as well as a boundary term consisting of interactions between the electron and the nuclear worldline,

$$S_b = -\int d\tau \sqrt{-\dot{y}^2}\left(M + h\,|\Psi(y)|^2 + \dots\right). \tag{2.2}$$

In (2.1), $V(r)$ may be some potential sourced by the point-particle, and the dots represent terms of higher powers in kR. In what follows, we choose $V(r) = \frac{g}{r^2}$. On its own, the excessive singularity of the inverse-square potential leads to ambiguities regarding the boundary condition at the origin [16]. Considerations of the self-adjointness of the Hamiltonian are often used to help resolve this difficulty, in particular by means of self-adjoint extensions [17–23]. A PPEFT however provides a natural solution to this problem by tying the near-source boundary condition unambiguously to the high-energy physics of the point particle, which may or may not lead to a self-adjoint Hamiltonian for the light degrees of freedom (for an example where probability for the bulk field is lost see [13], and the discussion in chapter 7, below). For a single bulk species this was considered in detail in Burgess et al. [5], and in particular it was shown that the inverse-square potential leads to a non-trivial renormalization of the point-particle coupling h. We briefly recall the results of that calculation below, and in the next section we will ask whether or not similar behavior is seen in the flavor-changing coupling.

Now through (2.2), there are couplings on the world-line $y^\mu(\tau)$ of the nucleus (parameterized by its proper time τ, so that $\dot{y}^\mu := \frac{dy^\mu}{d\tau}$ is the 4-velocity of the nucleus). The first term $\sqrt{-\dot{y}^2}M$ can be recognized as the usual action for a point-particle [24], while the second term is the lowest-order (in powers of length) coupling between the electron and the nucleus, with the dots representing interactions of higher order in kR. For a spherically symmetric nucleus, the coupling h is a constant.

For simplicity, and to emphasize the value of the point-particle interactions, we work in the limit of infinite nuclear mass, where $y^\mu = (t, 0, 0, 0)$ is the center-of-mass frame, and $\tau = t$. This amounts to neglecting nuclear recoil, but that can be included by explicitly tracking the dynamics of $y^\mu(\tau)$. Requiring the action to remain stationary with respect to variations of Ψ^* that vanish on the boundary yields the usual Schrödinger equation in the bulk

$$\left(i\partial_t + \frac{\nabla^2}{2m} - \frac{g}{r^2}\right)\Psi = 0, \tag{2.3}$$

while including variations on the boundary leads to the boundary condition

$$\lim_{\epsilon\to 0} 4\pi\epsilon^2\partial_\epsilon\Psi_\ell = \lim_{\epsilon\to 0} 2mh\Psi_\ell(\epsilon), \tag{2.4}$$

which defines $\partial_\epsilon := \partial_r|_\epsilon$, Ψ_ℓ as the ℓ^{th} eigenfunction of angular momentum. However, it is typically the case that one cannot carry out the limit in (2.4)—indeed, in our effective theory, $\epsilon \to 0$ is the UV regime we do not claim to understand anyway. The solution to this problem is to replace the point-particle action (2.2) with a boundary action defined on the surface of a ball $\mathcal{B}_\epsilon$ of radius ϵ centered at the world-line of the point-particle (see **Appendix A** of [5]). In the center of mass frame of reference, this has the form:

$$\mathcal{S}_\mathcal{B} = -\frac{1}{4\pi}\int_{\partial\mathcal{B}_\epsilon} d^2\Omega \left(M + \sum_\ell h_\ell|\Psi_\ell(\epsilon)|^2\right) \tag{2.5}$$

and yields the revised boundary condition

$$4\pi\epsilon^2\partial_\epsilon\Psi_\ell = 2mh_\ell\Psi_\ell(\epsilon). \tag{2.6}$$

Here, h has been replaced by a different coupling h_ℓ to each angular momentum mode of the bulk particle (for more on why this is the case, see [13]). With the limit now gone, the fictitious scale ϵ appears explicitly in the boundary condition for the bulk field, and so runs the risk of appearing in physical quantities. The way around this is to observe that h_ℓ is not itself a

[2]We use a mostly plus metric, and work in units such that $\hbar = c = 1$.

physical quantity, and so must be renormalized with ϵ such that all physical quantities in the boundary condition (2.6) remain ϵ-independent. We explicitly compute this running next.

The bulk equations (2.3) (now defined only outside $\mathcal{B}_\epsilon$) are solved by

$$\Psi = e^{-iEt}\left(C_+\psi_+ + C_-\psi_-\right)Y_{\ell,m}, \tag{2.7}$$

where E is the electron energy, $Y_{\ell,m}$ are the usual spherical harmonics, and the mode functions are

$$\psi_\pm(\rho) := \rho^{\frac{1}{2}(-1\pm\zeta)}e^{-\rho/2}\mathcal{M}\left[\frac{1}{2}\left(1\pm\zeta\right), 1\pm\zeta; \rho\right] \tag{2.8}$$

which defines $k^2 := 2mE$, $\rho := 2ikr$, and $\zeta := \sqrt{(2\ell+1)^2 - 8mg}$. For simplicity, in this paper we will restrict to the case $mg \leq 1/8$ so that ζ is always real. Taking the small $k\epsilon$ limit of (2.8), the boundary condition determines the renormalization-group flow of the coupling h_ℓ through

$$\hat{\lambda} = \frac{1 - \frac{C_-}{C_+}(2ik\epsilon)^{-\zeta}}{1 + \frac{C_-}{C_+}(2ik\epsilon)^{-\zeta}} = \frac{1 + (\epsilon/\epsilon_\star)^{-\zeta}}{1 - (\epsilon/\epsilon_\star)^{-\zeta}}, \tag{2.9}$$

where $\hat{\lambda} := \frac{1}{\zeta}(mh/\pi\epsilon + 1)$ (we drop the subscript ℓ for convenience), $y := \mathrm{sgn}(|\hat{\lambda}| - 1)$ defines a renormalization-group trajectory, and $\epsilon_\star$ is an RG-invariant length scale, both determined by the physical quantity

$$\frac{C_-}{C_+} = -y(2ik\epsilon_\star)^\zeta. \tag{2.10}$$

Physical quantities like scattering cross-sections and bound-state energies are directly related to the ratio C_-/C_+, and so through (2.10) directly to the quantity $\epsilon_\star$, which is fundamentally a property of the source. The usefulness of the inverse-square potential lies in how it can force non-trivial RG behavior upon the point-particle coupling. For example, the running (2.9) has an "infrared" fixed point of $+1$ when $\epsilon/\epsilon_\star \to \infty$, which corresponds to $\epsilon_\star \to 0$. For the s-wave in the absence of an inverse-square potential, $\zeta(\ell = 0) = 1$ and this would be equivalent to vanishing point-particle coupling, but if the strength of the inverse-square potential $g \neq 0$, then the fixed point is driven away from a vanishing point-particle coupling.

In the next section, we generalize all of this to a bulk system composed of multiple species of particles (though for concreteness, we specialize to two species). We see how most of the above follows through identically, but the presence of boundary terms that mix flavors adds a new degree of complexity to the problem, introducing a new point-particle coupling which runs differently from (2.9) and opening the door to flavor-changing reactions.

3. MULTI-SPECIES ACTION AND BULK FIELD EQUATIONS

The simplest extension of the basic point-particle action (2.2) to multiple particles is a non-diagonal quadratic one:

$$S_b^{(\mathrm{MP})} = -\int d\tau\sqrt{-\dot{y}^2}\left[M + \Psi_i^* h_{ij}\Psi_j + \dots\right] \tag{3.1}$$

where now there are N complex scalar Schroödinger fields Ψ_i, and summation over the species index is implied. The bulk action is taken to diagonalize the momentum operator, so flavor mixing only happens at the point particle, and the bulk action is simply N copies of (2.1):

$$\begin{aligned} S_B^{(\mathrm{MP})} &= \sum_{i=1}^{N}\int d^4x\left\{\frac{i}{2}\left(\Psi_i^*\partial_t\Psi_i - \Psi_i\partial_t\Psi_i^*\right)\right. \\ &\left. -\frac{1}{2m_i}|\nabla\Psi_i|^2 - V(r)|\Psi_i|^2\right\}. \end{aligned} \tag{3.2}$$

For concreteness, we will work with only $N = 2$ species of particles. Our interest is in single particle states, so we restrict to the single-particle sector, for which the Hilbert space is $\mathcal{H} = \mathbb{C}\oplus\mathcal{H}_1\oplus\mathcal{H}_2$ (where $\mathcal{H}_i$ is the Hilbert space for particle i). On this space, the Schrödinger operator $i\partial_t + \frac{\nabla^2}{2m_i} - \frac{g}{r^2}$ is diagonal. Writing the total wavefunction $\Psi = \begin{pmatrix}\Psi_1\\ \Psi_2\end{pmatrix}$, the equations of motion read

$$\begin{bmatrix} i\partial_t + \frac{\nabla^2}{2m_1} - \frac{g}{r^2} & 0 \\ 0 & i\partial_t + \frac{\nabla^2}{2m_2} - \frac{g}{r^2}\end{bmatrix}\begin{bmatrix}\Psi_1\\ \Psi_2\end{bmatrix} = 0. \tag{3.3}$$

The time-dependence is easily solved using separation-of-variables: $\Psi = e^{-iEt}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}$. Then we find

$$\begin{bmatrix} k_1^2 + \nabla^2 - \frac{g}{r^2} & 0 \\ 0 & k_2^2 + \nabla^2 - \frac{g}{r^2}\end{bmatrix}\begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix} = 0, \tag{3.4}$$

which defines the wavenumbers $k_i := \sqrt{2m_iE}$ (real for continuum states and imaginary for bound states).

Away from the origin, (3.4) is solved exactly as in the single-species problem, and a natural choice of basis for the solutions is

$$\mathcal{B} = \left\{\begin{pmatrix}\psi_1\\ 0\end{pmatrix}, \begin{pmatrix}0\\ \psi_2\end{pmatrix}\right\}, \tag{3.5}$$

where

$$\psi_i = \left(C_{i+}\psi_+(\ell_i; 2ik_ir) + C_{i-}\psi_-(\ell_i; 2k_ir)\right)Y_{\ell_i m_i}. \tag{3.6}$$

and

$$\psi_\pm(\ell;\rho) := \rho^{\frac{1}{2}(-1\pm\zeta_i)}e^{-\rho/2}\mathcal{M}\left[\frac{1}{2}\left(1\pm\zeta_i\right), 1\pm\zeta_i; \rho\right] \tag{3.7}$$

with $\rho := 2ikr$, and $\zeta_i := \sqrt{(2\ell+1)^2 - 8m_i g}$, and Y_{ℓ_i,m_i} the usual spherical harmonics, as in the single-particle example.

The constants $C_{i\pm}$ are solved by considering the boundary conditions in the problem, typically finiteness at large- and small-r, but for scattering problems the large-r BC is specific to the setup (since it depends on the presence or otherwise of incident particles). In a PPEFT, the small-r boundary condition is derived from the boundary action, which we describe next.

4. BOUNDARY CONDITIONS

In analogy with the single-particle system, we determine the small-r boundary condition by varying the point-particle action (3.1) directly [including the boundary terms in the variation of the bulk action (3.2)]. The resulting small-r boundary conditions are a simple generalization of (2.6):

$$4\pi\epsilon^2\partial_\epsilon\Psi = 2\mathbf{mh}\Psi(\epsilon), \tag{4.1}$$

again using $\Psi = e^{-iEt}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}$ and as in section 2, we define $\partial_\epsilon := \partial_r|_\epsilon$ (and we drop the angular momentum label on $\mathbf{h}$ as above). Here $\mathbf{m}$ and $\mathbf{h}$ are the mass and point-particle coupling matrices (respectively), so that in components,

$$4\pi\epsilon^2\partial_\epsilon\psi_1 - 2m_1h_{11}\psi_1(\epsilon) - 2m_1h_{12}\psi_2(\epsilon) = 0 \qquad \text{and} \tag{4.2a}$$

$$4\pi\epsilon^2\partial_\epsilon\psi_2 - 2m_2h_{22}\psi_2(\epsilon) - 2m_2h_{21}\psi_1(\epsilon) = 0. \tag{4.2b}$$

Notice that the explicit ϵ-dependence of (4.2) again indicates that the point-particle couplings h_{ij} *must* be renormalized with ϵ whenever Ψ or $\partial_\epsilon\Psi$ diverge for small argument, in order for the boundary condition to be compatible with the bulk equations of motion.

The boundary condition then serves two distinct purposes: (i) solving for the integration constants in Ψ tells us how they (and correspondingly physical quantities) depend on the point-source physics, and (ii) isolating for the couplings h_{ij} then tells us how exactly each coupling flows with ϵ to ensure the physical integration constants do not. Clearly though, with four possible degrees of freedom in $\mathbf{h}$ and four integration constants in Ψ, the two equations in (4.2) are insufficient by themselves. In the next sections we invoke physical arguments to resolve this predicament, and separately tackle both problems (i) and (ii).

4.1. Solving for Integration Constants

The most obvious place to look for additional constraints is at another boundary. In spherical coordinates, this amounts to looking at the asymptotic behavior of Ψ as $r\to\infty$. However, the asymptotic behavior of the system is not unique, and is a very situation-dependent property. Since our interest in this paper is in catalysis of flavor violation, it is most pertinent to study scattering states.

First, focus on scattering $\Psi_1 \to \Psi_j$. In this case, asymptotically we need (see **Appendix A.2** for a review of multi-species scattering) $\psi_1(r\to\infty) \to e^{ik_1z} + f_{11}(\theta,\psi)\frac{e^{ik_1r}}{k_1r}$ as usual, and now also $\psi_2(r\to\infty)\to f_{12}(\theta,\psi)\frac{e^{ik_2r}}{k_2r}$. Notice that both boundary conditions and the equations of motion are linear in Ψ, so we may divide through by one integration constant. For incident particle 1, we will choose to divide through by C_{1+}, and we will define

$$C_{11} := \frac{C_{1-}}{C_{1+}}, \quad \text{and} \quad C_{12} := \frac{C_{2-}}{C_{1+}} \qquad (1\to X \text{ scattering}), \tag{4.3}$$

and eliminating the infalling wave in ψ_2 fixes $C_{2+} = R\,C_{2-}$ with

$$R := -\frac{\Gamma(1-\zeta/2)}{\Gamma(1+\zeta/2)}2^{-2\zeta}e^{-i\pi\zeta} \tag{4.4}$$

As we will see in the section 5, C_{11} and C_{12} are directly related to the physical cross-sections for $\Psi_1 \to \Psi_1$ and $\Psi_1\to\Psi_2$ scattering.

Using the definitions (4.3) and (4.4) in the small-r boundary condition (4.2) yields

$$4\pi\epsilon^2\partial_\epsilon(\psi_{1+} + C_{11}\psi_{1-}) - h_{11}(\psi_{1+} + C_{11}\psi_{1-}) - h_{12}C_{12}(R\,\psi_{2+} + \psi_{2-}) = 0 \text{ and} \tag{4.5a}$$

$$4\pi\epsilon^2 C_{12}\partial_\epsilon(R\,\psi_{2+} + \psi_{2-}) - h_{22}C_{12}(R\,\psi_{2+} + \psi_{2-}) - h_{21}(\psi_{1+} + C_{11}\psi_{1-}) = 0, \tag{4.5b}$$

Finally, in terms of integration constants the boundary condition (4.5) is now a system of two equations for two unknowns, so using the small-r forms of the bulk modes (3.7),

$$\psi_\pm(\ell;\epsilon) \approx (2ik\epsilon)^{\frac{1}{2}(-1\pm\zeta)} \implies \left.\frac{\partial}{\partial r}\right|_\epsilon \psi_\pm(\ell;\rho) \approx ik(-1\pm\zeta)(2ik\epsilon)^{\frac{1}{2}(-3\pm\zeta)}, \tag{4.6}$$

it is found (see **Appendix B** for details of the calculation) that the integration constants for this system are related to the source physics through

$$C_{11} = -(2ik_1\epsilon)^{\zeta_1}\frac{\widehat{\mathcal{N}}_1}{\widehat{\mathcal{D}}} \qquad \text{and}$$

$$C_{12} = (2ik_1\epsilon)^{\zeta_1/2}(2ik_2\epsilon)^{\zeta_2/2}\sqrt{\frac{m_2k_2\zeta_1}{m_1k_1\zeta_2}}\frac{\hat{\lambda}_{21}}{\widehat{\mathcal{D}}},$$

where

$$\widehat{\mathcal{N}}_1 : = 4\widehat{\lambda}_{12}\widehat{\lambda}_{21} - \left[\widehat{\lambda}_{11}-1\right]\left[\widehat{\lambda}_{22}+1\right], \qquad \text{and}$$
$$\widehat{\mathcal{D}} : = 4\widehat{\lambda}_{12}\widehat{\lambda}_{21} - \left[\widehat{\lambda}_{11}+1\right]\left[\widehat{\lambda}_{22}+1\right], \tag{4.7}$$

and the following convenient re-definitions have been made:

$$\widehat{\lambda}_{11} := \frac{1}{\zeta_1}\left(\frac{m_1h_{11}}{\pi\epsilon}+1\right), \qquad \widehat{\lambda}_{22} := \frac{1}{\zeta_2}\left(\frac{m_2h_{22}}{\pi\epsilon}+1\right), \text{ and,} \tag{4.8}$$

$$\widehat{\lambda}_{12} := \frac{h_{12}\sqrt{m_1 m_2}}{2\pi\epsilon\sqrt{\zeta_1\zeta_2}}, \qquad \widehat{\lambda}_{21} := \frac{h_{21}\sqrt{m_1 m_2}}{2\pi\epsilon\sqrt{\zeta_1\zeta_2}}. \tag{4.9}$$

Of course, the choice to make particle 1 the incident particle was not forced upon us, and with foresight to the next sections, we also compute the quantities involved in scattering $\Psi_2 \to \Psi_i$. Fortunately, this is exactly the $1 \leftrightarrow 2$ inversion of the $1 \to X$ scattering above, so we can immediately write:

$$\begin{aligned} 4\pi\epsilon^2 C_{12}\partial_\epsilon\,(R\psi_{2+} + \psi_{2-}) - \quad & h_{22}C_{12}\,(R\psi_{2+} + \psi_{2-}) \\ - \quad & h_{21}\,(\psi_{1+} + C_{11}\psi_{1-}) = 0 \quad \text{and} \end{aligned} \tag{4.10a}$$

$$\begin{aligned} 4\pi\epsilon^2\partial_\epsilon\,(\psi_{1+} + C_{11}\psi_{1-}) - \quad & h_{11}\,(\psi_{1+} + C_{11}\psi_{1-}) \\ - \quad & h_{12}C_{12}\,(R\psi_{2+} + \psi_{2-}) = 0, \end{aligned} \tag{4.10b}$$

where as above we have defined

$$C_{22} := \frac{C_{2-}}{C_{2+}}, \quad \text{and} \quad C_{21} := \frac{C_{1-}}{C_{2+}} \qquad (2 \to X \text{ scattering}), \tag{4.11}$$

now with $C_{1+} = R\,C_{1-}$. Solving for the integration constants similarly yields

$$\begin{aligned} C_{22} &= -(2ik_2\epsilon)^{\zeta_2}\frac{\widehat{\mathcal{N}}_2}{\widehat{\mathcal{D}}} \qquad \text{and} \\ C_{21} &= (2ik_1\epsilon)^{\zeta_1/2}(2ik_2\epsilon)^{\zeta_2/2}\sqrt{\frac{m_1k_1\zeta_2}{m_2k_2\zeta_1}}\frac{\hat{\lambda}_{12}}{\widehat{\mathcal{D}}}, \end{aligned} \tag{4.12}$$

4.2. Renormalization-Group Flows and Invariants

Next we move on to teasing out of the boundary condition (4.2) exactly how the couplings h_{ij} must be renormalized with ϵ to keep physical quantities independent of the regulator. One way to do so would be to differentiate (4.7) and (4.12) with respect to ϵ while holding the (physical) integration constants fixed, and solve the resulting differential equations. This approach turns out to be very difficult however, since the equations are highly coupled and tough to disentangle. Notice however that it is important to have knowledge of both $1 \to X$ and $2 \to X$ scattering to solve for all the elements of **h**. This is not a coincidence. A unitary system requires a real action, which is enforced by the condition that **h** is Hermitian. At the same time, a unitary S-matrix for an N-species system has N^2 real degrees of freedom, which is the same dimension as an $N \times N$ Hermitian matrix. Consequently, connecting the point-particle couplings to physical quantities requires knowledge of the entire S-matrix, and so in our case must involve both $1 \to X$ scattering and $2 \to X$ scattering. Lastly, one final simplification can be made by observing that the phase of h_{12} can be removed by a field redefinition, so for the special case of a two-species system we only have to deal with a real matrix of point-particle couplings.

The easiest approach to solving for the flows of the couplings h_{ij} is to go back to the boundary conditions (4.5) and (4.10) for both $1 \to X$ and $2 \to X$ systems and solve directly for the individual elements of **h**. This inversion is done in detail in **Appendix C**, and using the small-r form (4.6), the point-particle couplings must take the following forms as functions of the regulator ϵ.

$$\widehat{\lambda}_{11} = \frac{(1 - C_{11}(2ik_1\epsilon)^{-\zeta_1})(1 + C_{22}(2ik_2\epsilon)^{-\zeta_2}) + C_{21}C_{12}(2ik_1\epsilon)^{-\zeta_1}(2ik_2\epsilon)^{-\zeta_2}}{(1 + C_{11}(2ik_1\epsilon)^{-\zeta_1})(1 + C_{22}(2ik_2\epsilon)^{-\zeta_2}) - C_{21}C_{12}(2ik_1\epsilon)^{-\zeta_1}(2ik_2\epsilon)^{-\zeta_2}}, \tag{4.14a}$$

$$\widehat{\lambda}_{12} = \sqrt{\frac{m_2\zeta_1}{m_1\zeta_2}}\frac{C_{21}\left(\frac{k_1}{k_2}\right)^{-1/2}(2ik_1\epsilon)^{-\zeta_1/2}(2ik_2\epsilon)^{-\zeta_2/2}}{(1 + C_{11}(2ik_1\epsilon)^{-\zeta_1})(1 + C_{22}(2ik_2\epsilon)^{-\zeta_2}) - C_{21}C_{12}(2ik_1\epsilon)^{-\zeta_1}(2ik_2\epsilon)^{-\zeta_2}}, \tag{4.14b}$$

$$\widehat{\lambda}_{21} = \sqrt{\frac{m_1\zeta_2}{m_2\zeta_1}}\frac{C_{12}\left(\frac{k_2}{k_1}\right)^{-1/2}(2ik_1\epsilon)^{-\zeta_1/2}(2ik_2\epsilon)^{-\zeta_2/2}}{(1 + C_{11}(2ik_1\epsilon)^{-\zeta_1})(1 + C_{22}(2ik_2\epsilon)^{-\zeta_2}) - C_{21}C_{12}(2ik_1\epsilon)^{-\zeta_1}(2ik_2\epsilon)^{-\zeta_2}}, \tag{4.14c}$$

$$\widehat{\lambda}_{22} = \frac{(1 + C_{11}(2ik_1\epsilon)^{-\zeta_1})(1 - C_{22}(2ik_2\epsilon)^{-\zeta_2}) + C_{21}C_{12}(2ik_1\epsilon)^{-\zeta_1}(2ik_2\epsilon)^{-\zeta_2}}{(1 + C_{11}(2ik_1\epsilon)^{-\zeta_1})(1 + C_{22}(2ik_2\epsilon)^{-\zeta_2}) - C_{21}C_{12}(2ik_1\epsilon)^{-\zeta_1}(2ik_2\epsilon)^{-\zeta_2}}, \tag{4.14d}$$

where now

$$\widehat{\mathcal{N}}_2 := 4\widehat{\lambda}_{12}\widehat{\lambda}_{21} - \left[\widehat{\lambda}_{11} + 1\right]\left[\widehat{\lambda}_{22} - 1\right]. \tag{4.13}$$

It is important to note that the C_{ij} integration constants are fundamentally different, as they are determined by different asymptotic boundary conditions and correspond to different physics. In section 5 we will see exactly how they relate to the physical cross-sections, but having defined them all separately is already important at the level of renormalizing the point-particle couplings, which we do next.

using the definitions (4.9).

Equations (4.14) (together with (4.7), (4.12), (2.10), and past work [8]) suggests the integration constants can each be characterized by a unique RG-invariant length-scale. To see how this works, define the scales ϵ_1, ϵ_2, and ϵ_3 by the following relations:

$$C_{11} = -y_1(2ik_1\epsilon_1)^{\zeta_1}, \qquad C_{22} = -y_2(2ik_2\epsilon_2)^{\zeta_2},$$

$$\text{and} \quad C_{12} = \frac{m_2k_2\zeta_1}{m_1k_1\zeta_2}C_{21} = y_3\sqrt{\frac{m_2k_2\zeta_1}{m_1k_1\zeta_2}}(2ik_1\epsilon_3)^{\zeta_1/2}(2ik_2\epsilon_3)^{\zeta_2/2}, \tag{4.15}$$

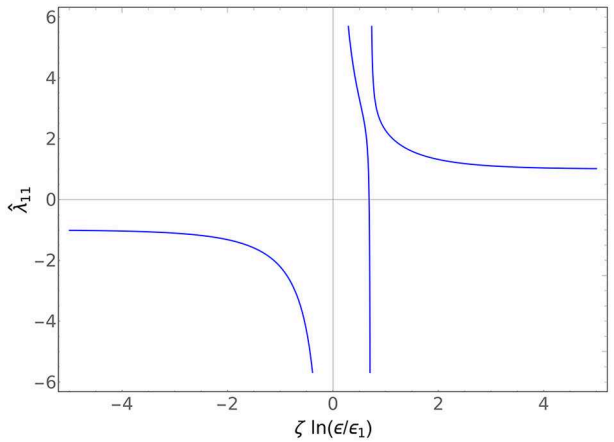

FIGURE 1 | Plot of $\widehat{\lambda}_{11}$ vs $\zeta \ln(\epsilon/\epsilon_1)$ for $\zeta_1 = \zeta_2$, $y_1 = y_2 = +1$, and $(\epsilon_2/\epsilon_1)^\zeta = 2$ and $(\epsilon_3/\epsilon_1)^\zeta = 0.02$. The fascinating second pole arises in certain limits of the ratio of ϵ_1 to ϵ_2 and ϵ_3. In the limit $\epsilon_3 \to 0$, this reduces to the classic single-particle RG.

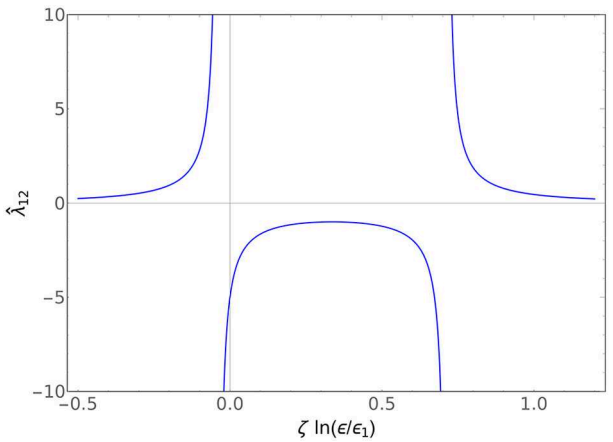

FIGURE 2 | Plot of $\widehat{\lambda}_{12}$ vs $\zeta \ln(\epsilon/\epsilon_1)$ for $\zeta_1 = \zeta_2$, $y_1 = y_2 = y_3 = +1$, and $(\epsilon_2/\epsilon_1)^\zeta = 2$ and $(\epsilon_3/\epsilon_1)^\zeta = 0.02$.

where $y_i = \pm 1$ defines a particular class of flow. In terms of these scales, the running equations are significantly simpler:

$$\widehat{\lambda}_{11} = \frac{\left(1 + y_1\,(\epsilon/\epsilon_1)^{-\zeta_1}\right)\left(1 - y_2\,(\epsilon/\epsilon_2)^{-\zeta_2}\right) + (\epsilon/\epsilon_3)^{-(\zeta_1+\zeta_2)}}{\left(1 - y_1\,(\epsilon/\epsilon_1)^{-\zeta_1}\right)\left(1 - y_2\,(\epsilon/\epsilon_2)^{-\zeta_2}\right) - (\epsilon/\epsilon_3)^{-(\zeta_1+\zeta_2)}}, \tag{4.16a}$$

$$\widehat{\lambda}_{12} = \widehat{\lambda}_{21} = \frac{y_3\,(\epsilon/\epsilon_3)^{-(\zeta_1+\zeta_2)/2}}{\left(1 - y_1\,(\epsilon/\epsilon_1)^{-\zeta_1}\right)\left(1 - y_2\,(\epsilon/\epsilon_2)^{-\zeta_2}\right) - (\epsilon/\epsilon_3)^{-(\zeta_1+\zeta_2)}}, \tag{4.16b}$$

$$\widehat{\lambda}_{22} = \frac{\left(1 - y_1\,(\epsilon/\epsilon_1)^{-\zeta_1}\right)\left(1 + y_2\,(\epsilon/\epsilon_2)^{-\zeta_1}\right) + (\epsilon/\epsilon_3)^{-(\zeta_1+\zeta_2)}}{\left(1 - y_1\,(\epsilon/\epsilon_1)^{-\zeta_1}\right)\left(1 - y_2\,(\epsilon/\epsilon_2)^{-\zeta_2}\right) - (\epsilon/\epsilon_3)^{-(\zeta_1+\zeta_2)}}, \tag{4.16c}$$

An example of $\widehat{\lambda}_{11}$ and $\widehat{\lambda}_{22}$ is plotted in **Figure 1**, and an example of $\widehat{\lambda}_{12}$ is plotted in **Figure 2**. All the couplings flow to fixed points in the ultraviolet ($\epsilon/\epsilon_i \to 0$) and the infrared ($\epsilon/\epsilon_i \to \infty$). The diagonal couplings $\widehat{\lambda}_{11}$ and $\widehat{\lambda}_{22}$ both flow to -1 in the UV and $+1$ in the IR, exactly as the single-particle flow does, while the off-diagonal $\widehat{\lambda}_{12}$ flows to vanishing coupling in both the cases. This says something reasonable: the system is perfectly content to live in a world where there is no species mixing, regardless of the existence of the inverse-square potential. However, if the species do mix, then the strength of that mixing depends on the scale it is measured at, with the flow given by (4.16b).

Interestingly, all three flows share a common denominator, which can always be factorized. When $\zeta_1 = \zeta_2 =: \zeta$, the zeroes of the denominator lie at

$$\epsilon_a^\zeta = \frac{1}{2}\left(y_2\epsilon_2^\zeta + y_1\epsilon_1^\zeta \pm \sqrt{\left(y_1\epsilon_1^\zeta - y_2\epsilon_2^\zeta\right)^2 + 4\epsilon_3^{2\zeta}}\right), \tag{4.17}$$

so there is at least one asymptote in all the flows as long as $y_2\epsilon_2^\zeta + y_1\epsilon_1^\zeta > 0$. Indeed, the only regime where there is *no* asymptote is where $-(y_2\epsilon_2^\zeta + y_1\epsilon_1^\zeta) > \sqrt{\left(y_1\epsilon_1^\zeta - y_2\epsilon_2^\zeta\right)^2 + 4\epsilon_3^{2\zeta}} > 0$.

The practicality of this framework lies in how the point-particle couplings [and in particular their RG-invariants (4.15)] inform physical quantities, like scattering cross-sections, and we investigate this next.

5. SCATTERING AND CATALYSIS OF FLAVOR VIOLATION

To see how the nuclear properties enter into macroscopic quantities, and in particular how the point-particle can induce a violation of bulk flavor-conservation, we proceed to compute the elements of the scattering matrix. In particular, it will be shown that the low-energy *s*-wave "elastic" ($\Psi_i \to \Psi_i$) scattering is as usual independent of incoming momentum, and ϵ_i plays the role of the scattering length. Meanwhile, the flavor-violating "inelastic" cross-section is uniquely characterized by ϵ_3, which can be thought of as an effective scattering length for flavor violation. Moreover, the inelastic cross-section goes as $k_{\text{out}}/k_{\text{in}}$. This ratio is a constant for Schrödinger particles, but for Klein-Gordon fields (such as is appropriate for, say, incident pions) the ratio has a dependence on the incoming momentum, and that dependence takes on a variety of qualitatively different forms determined by the size of $k_{\text{in}}^2/|m_1^2 - m_2^2|$. Of particular interest is the case where the incoming particle's mass is greater than the outgoing particle's mass, and the incoming particle's momentum is small compared to the mass gap, in which case the flavor-violating cross-section is catalyzed, and goes as $1/k_{\text{in}}$ (although such a setup would certainly be hard to realize in practice).

Following the **Appendix A.2**, we need to identify the scattering matrix elements $S_{ij}^{(\ell)}$ in terms of C_{ij}.

5.1. Elastic Scattering ($\psi_i \to \psi_i$)

First consider elastic scattering of ψ_1. This is the case where the measured particle is the same as the incoming particle, so the asymptotic form of ψ_1 contains an incoming plane wave and an outgoing spherical wave:

$$\psi_1^{\text{Ans}}(r\to\infty)\to\mathcal{C}\left(e^{ik_1 z}+f_{11}(\theta,\psi)\frac{e^{ik_1 r}}{r}\right). \tag{5.1}$$

Starting from the general form (3.6) for particle 1,

$$\psi_1=(C_{1+}\psi_{1+}+C_{1-}\psi_{1-})Y_{\ell_1,m_1}, \tag{5.2}$$

the large-r limit is (taking the asymptotic limit of the confluent hypergeometric function)

$$\psi_1(r\to\infty)\to A_\ell\frac{e^{i(k_1 r-\ell\pi/2)}}{2ik_1 r}+B_\ell\frac{e^{-i(k_1 r-\ell\pi/2)}}{2ik_1 r}, \tag{5.3}$$

where

$$\begin{aligned}A_\ell&=\left[\Gamma\left(1+\frac{1}{2}\zeta_1\right)2^{\zeta_1}C_{1+}+\Gamma\left(1-\frac{1}{2}\zeta_1\right)2^{-\zeta_1}C_{1-}\right]\frac{e^{i\pi\ell/2}}{\sqrt{\pi}},\quad\text{and}\\ B_\ell&=\left[\Gamma\left(1+\frac{1}{2}\zeta_1\right)2^{\zeta_1}C_{1+}+\Gamma\left(1-\frac{1}{2}\zeta_1\right)2^{-\zeta_1}e^{-i\pi\zeta_1}C_{1-}\right]\frac{e^{i(1+\zeta_1-\ell)\pi/2}}{\sqrt{\pi}}.\end{aligned} \tag{5.4}$$

Matching to the asymptotic form (5.1), allows us to identify (see 12.1) the overall normalization

$$\begin{aligned}\mathcal{C}\;=\;&\frac{(-1)^{\ell+1}}{2\pi\sqrt{(2\ell+1)}}\left[\Gamma\left(1+\frac{1}{2}\zeta_1\right)2^{\zeta_1}C_{1+}\right.\\&\left.+\Gamma\left(1-\frac{1}{2}\zeta_1\right)2^{-\zeta_1}e^{-i\pi\zeta_1}C_{1-}\right]e^{i(1+\zeta_1)\pi/2},\end{aligned} \tag{5.5}$$

and the scattering matrix element

$$\begin{aligned}S_{11}^{(\ell)}&=-\frac{A_\ell}{B_\ell}\\&=\frac{\left[\Gamma\left(1+\zeta_1/2\right)+\Gamma\left(1-\zeta_1/2\right)2^{-2\zeta_1}C_{11}\right]}{\left[\Gamma\left(1+\zeta_1/2\right)+\Gamma\left(1-\zeta_1/2\right)2^{-2\zeta_1}e^{-i\pi\zeta_1}C_{11}\right]}e^{i(2\ell+1-\zeta_1)\pi/2}.\end{aligned} \tag{5.6}$$

Our interest is in the regime where $k_i\epsilon$ is small, so the s-wave is the dominant contribution to the cross-section. In the s-wave, $\zeta_1=\zeta_{1s}:=\sqrt{1-8m_1 g}$, and the cross-section is (A.9), exactly as in Burgess et al. [6]:

$$\sigma_s^{(1\to1)}=\frac{\pi}{k_1^2}|S_{11}^{(0)}|^2=\frac{\pi}{k_1^2}\left|\frac{1-\mathcal{A}e^{i\pi\zeta_{1s}/2}}{1-\mathcal{A}e^{-i\pi\zeta_{1s}/2}}\right|^2 \tag{5.7}$$

where

$$\mathcal{A}:=e^{-i\pi\zeta_1/2}2^{-2\zeta_1}C_{11}\frac{\Gamma[1-\frac{1}{2}\zeta_1]}{\Gamma[1+\frac{1}{2}\zeta_1]}=y_1\left(\frac{k_1\epsilon_1}{2}\right)^{\zeta_1}\frac{\Gamma[1-\frac{1}{2}\zeta_1]}{\Gamma[1+\frac{1}{2}\zeta_1]}. \tag{5.8}$$

[The second equality uses (4.15) to exchange the integration constants for the RG-invariant ϵ_1]. Of particular note is when there is no inverse-square potential, in which case $\zeta_{1s}=1$ and the cross-section reduces to

$$\sigma_s^{(1\to1)}=4\pi\epsilon_1^2\qquad(g=0), \tag{5.9}$$

which can be identified as the cross-section for scattering from a 3D δ-function potential (see for example [25] where our ϵ_1 corresponds to their $g/\sqrt{\pi}$). Elastic scattering for the second species $\psi_2\to\psi_2$ follows exactly the same procedure and is trivially the $1\leftrightarrow2$ inversion of (5.7) and (5.8).

$$\sigma_s^{(2\to2)}=4\pi\epsilon_2^2\qquad(g=0). \tag{5.10}$$

5.2. Flavor-Violating Scattering ($\psi_i \to \psi_j$, $i \neq j$)

So much for the ordinary scattering. Finally we compute the flavor-violating $\psi_1\to\psi_2$ cross-section, and see the point-particle catalysis in action. This time, there is no incoming flux of the particle to be measured, so the large-r ansatz is simply:

$$\psi_2^{\text{Ans}}(r\to\infty)\to\mathcal{C}f_2(\theta,\psi)\frac{e^{ik_2 r}}{r}. \tag{5.11}$$

where we have scaled out the same normalization factor $\mathcal{C}$, for convenience. The asymptotic form of the general solution for ψ_2 is exactly (5.3) subject to $1\leftrightarrow2$, so we can immediately observe the following. First, as was used in deriving the boundary conditions in section 4, $B_\ell=0$ so that $C_{2+}=RC_{2-}$, where as above

$$R:=-\frac{\Gamma(1-\zeta/2)}{\Gamma(1+\zeta/2)}2^{-2\zeta}e^{-i\pi\zeta}. \tag{5.12}$$

Following **Appendix A.2**, this time we identify the inelastic scattering element $S_{12}^{(\ell)}$ using (A.15)

$$\begin{aligned}S_{12}^{(\ell)}&=\frac{e^{-i\pi\ell/2}}{\sqrt{4\pi(2\ell+1)}}\frac{A_\ell}{\mathcal{C}}=\frac{\Gamma\left(1-\frac{1}{2}\zeta_2\right)}{2\pi\sqrt{(2\ell+1)}}\frac{C_{2-}}{\mathcal{C}}2^{-\zeta_2}(1-e^{-i\pi\zeta_2}),\\&=\frac{(-1)^{-\ell+1}}{2^{\zeta_1+\zeta_2-1}}\sin(\pi\zeta_2/2)e^{i\pi(\ell-\zeta_1-\zeta_2-1)/2}\frac{\Gamma\left(1-\frac{1}{2}\zeta_2\right)}{\Gamma\left(1+\frac{1}{2}\zeta_1\right)}\frac{C_{12}}{1-\mathcal{A}e^{-i\pi\zeta_1/2}}.\end{aligned} \tag{5.13}$$

where $\mathcal{A}$ is defined in (5.8).

Again, our interest is in the small $k_i\epsilon$ regime for which the s-wave dominates. We similarly define $\zeta_{2s}:=\sqrt{1-8m_2 g}$. Then the low-energy cross-section is (A.16),

$$\begin{aligned}\sigma_s^{(1\to2)}&=\frac{\pi}{k_1k_2}\frac{m_1}{m_2}\left|S_{12}^{(0)}\right|^2,\\&=\frac{4\pi}{2^{\zeta_1+\zeta_2}}\frac{k_1^{\zeta_1}k_2^{\zeta_2}}{k_1^2}\frac{\zeta_1}{\zeta_2}\sin^2(\pi\zeta_2/2)\frac{\epsilon_3^{\zeta_1+\zeta_2}}{|1-\mathcal{A}e^{-i\pi\zeta_1/2}|^2}\left(\frac{\Gamma\left(1-\frac{1}{2}\zeta_2\right)}{\Gamma\left(1+\frac{1}{2}\zeta_1\right)}\right)^2.\end{aligned} \tag{5.14}$$

As in the elastic case, the reverse scattering $\psi_2\to\psi_1$ is a simple matter of exchanging $1\leftrightarrow2$ in (5.14). In the absence

of an inverse-square potential ($\zeta_{is} = 1$), the cross-section (5.14) simplifies significantly.

$$\sigma_s^{1\to 2} = 4\pi \frac{k_2}{k_1}\epsilon_3^2 \qquad (g = 0). \tag{5.15}$$

On its own, this is an interesting enough result. The flavor-violating cross-section is non-zero only when the point-particle has non-trivial flavor-violating properties, as are encoded in ϵ_3. This is also the statement that flavor-violation only occurs if $h_{12} \neq 0$, since it is always true—regardless of the presence of an inverse-square potential—that $h_{12} = 0$ only when $\epsilon_3 = 0$[3].

A particularly interesting aspect of (5.15) is the factor of k_2/k_1. For Schrödinger particles, this is just a constant ($k_i = \sqrt{2m_i E} \implies k_2/k_1 = \sqrt{m_2/m_2}$). In section 6, we treat a Schrödinger particle interacting with a multi-state nucleus, in which case the final and initial momenta do differ non-trivially, but even at the level of two bulk species, more interesting dynamics can be seen just by treating the particles as relativistic Klein-Gordon fields. For relativistic fields, the cross-section takes the same general form as (5.15), except the momenta are relativistic: $k_i = \sqrt{\omega^2 - m_i^2}$, where ω is the energy of the system. Then $\omega^2 = k_i^2 + m_i^2$, so that

$$\frac{k_2}{k_1} = \frac{\sqrt{k_1^2 + (m_1^2 - m_2^2)}}{k_1}. \tag{5.16}$$

The cross-section therefore exhibits different qualitative behavior depending on how the incoming momentum k_1 relates to the (squared) mass gap $m_1^2 - m_2^2$. This can be broadly classified by 4 different regimes depending on the sign of $m_1^2 - m_2^2$ and the size of the ratio $r := k_1^2/|m_1^2 - m_2^2|$.

First, if the mass gap is positive, the only question is to the size of the ratio r. If $r \ll 1$, then $\sigma_s^{(1\to 2)} \sim k_1^{-1}$. This is the regime where the cross-section sees a low-energy enhancement similar to the well-known enhancement of absorptive cross-sections [26] (more on that in section 6). However, if $r \gg 1$, then the cross-section is roughly independent of the incoming momentum altogether. The cross-over between these regimes is plotted in **Figure 3**. These are indeed reasonable behaviors. If $m_1 > m_2$, and the incoming momentum is small compared to the mass difference, then the transition is to a lighter particle traveling faster, which is intuitively a more favorable process—the heavier incident particle has access to a larger phase-space than the lighter incident particle. If the mass difference is small compared to the incoming momentum, then the benefit of transitioning to a particle with a smaller mass is minimal, so the process is no more favorable than no transition. If instead the mass gap is negative, then there is a new regime. If $k_1^2 < m_2^2 - m_1^2$ (so if $r < 1$) there is in fact *no* scattering. This is certainly reasonable—if the incident particle did not have enough energy to create the rest mass of the second particle, then it cannot scatter into that particle (this is the threshold behavior described by [27, section 144]). If $r \gtrsim 1$, the incident momentum is just enough to create the second particle $k_1^2 = m_2^2 - m_1^2 + \delta$, then the cross-section goes as $\sqrt{\delta/(m_2^2 - m_1^2)}$. Since $k_2^2 = k_1^2 + m_1^2 - m_2^2 = \delta \ll m_2^2$, this is also the statement that the cross-section goes as v_2, the (non-relativistic) speed of the final state particle. Finally, if $r \gg 1$, the incident momentum greatly exceeds the mass gap and we again see the cross-section behave independently from k_1, as before. These momentum-dependences are plotted in **Figure 4**.

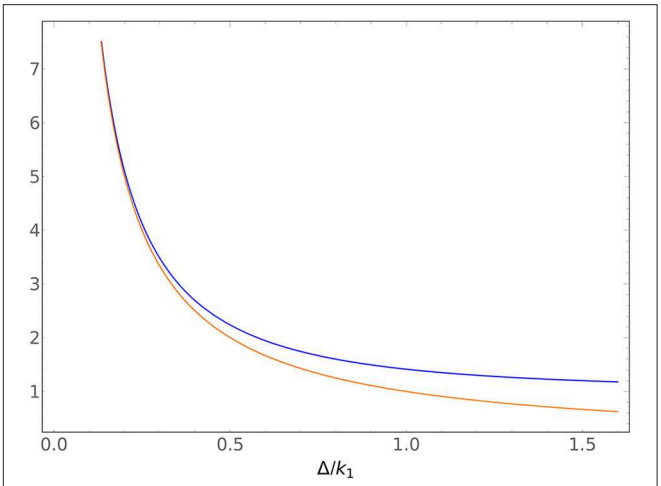

FIGURE 3 | Plot of the cross-over behavior in the k dependence of the inelastic cross-section for a Klein-Gordon particle conversion in units of Δ/k_1, where $\Delta = \sqrt{m_1^2 - m_2^2}$ and $m_1 > m_2$. The full function $\sqrt{1 + \Delta^2/k_1^2}$ is plotted in blue, and the simple inelastic behavior Δ/k_1 is plotted in orange. Notice the overlap for small Δ/k_1, and the strong enhancement for large momenta.

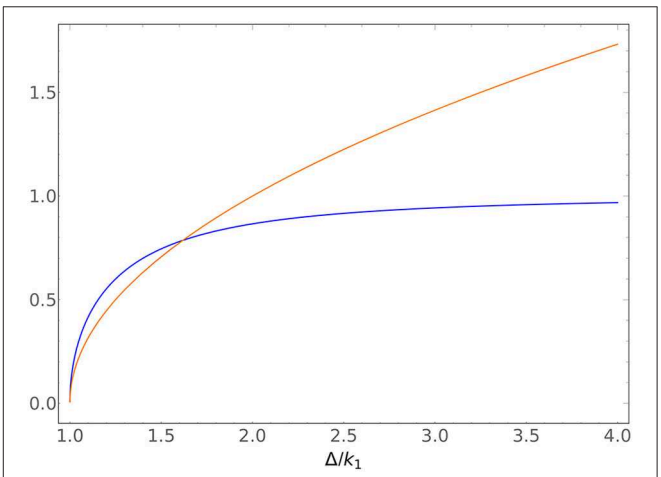

FIGURE 4 | Plot of the cross-over behavior in the k dependence of the inelastic cross-section for a Klein-Gordon particle conversion in units of Δ/k_1, where $\Delta = \sqrt{m_1^2 - m_2^2}$ and $m_2 > m_1$. The full function $\sqrt{1 - \Delta^2/k_1^2}$ is plotted in blue, and the simple inelastic behavior $\sqrt{\Delta/k_1 - 1}$ is plotted in orange. Notice the threshold cutoff at $\Delta/k_1 = 1$, as well as the approximate overlap for small Δ/k_1, and the strong suppression for large momenta.

[3] As noted in section 4.2, this is in contrast to the behavior of h_{11} and h_{22}, whose flows indicate that $\epsilon_1, \epsilon_2 \to 0$ is only consistent with $h_{11}, h_{22} \to 0$ when there is no inverse-square potential.

6. TRANSFER REACTIONS AND NUCLEAR STRUCTURE

In many cases, a reaction with a nucleus can change not only the incident particle, but also the nucleus. This can be the case even when scattering energies are low compared to the mass of the nucleus. For instance, the excitation energy of most real nuclei is on the order of MeV compared to their masses of order GeV [28]. A particularly interesting class of reactions that falls into this category is transfer reactions, where a composite particle (say a neutron) scatters off of a nucleus and exchanges a constituent particle (say a quark) with one of the valence nucleons, so that the outgoing particle is different (perhaps a proton) and so is the nucleus. While this work is not enough to describe a complete transfer reaction, we can make progress toward a complete description, and can at least describe the simpler process $\psi + N \rightarrow \psi + N^*$, where N is some nucleus and N^* is a long-lived excited state of that nucleus. The key observation to make is that there is essentially no difference between a system spanned by $\{\Psi_1 \otimes |N\rangle, \Psi_2 \otimes |N\rangle\}$ with $|N\rangle$ some nuclear state, and $\{\Psi \otimes |N_1\rangle, \Psi \otimes |N_2\rangle\}$ where $|N_i\rangle$ are distinct nuclear states. The only complexity lies in describing the different nuclear states in a point-particle EFT language.

Here we will sketch out the simplest point-particle action that includes a two-state nucleus coupled to a single bulk field, but a more detailed treatment of a PPEFT for a point-particle with internal degrees of freedom will be available in Zalavái et al. (in preparation). In addition to the single-species action (2.2), introduce an auxiliary grassmann-valued field T_i that satisfies the commutation relations of the generators of $\mathfrak{su}(2)$.

$$S_b^{2N} = -\int d\tau \sqrt{-\dot{y}^2}\,\left(M + iT_i\dot{T}^i - i\epsilon_{ijk}\Delta_i T_j T_k + h'|\Psi(y(\tau))|^2 - \epsilon_{ijk}g'_i T_j T_k |\Psi(y(\tau))|^2\right). \tag{6.1}$$

Here, Δ_i and g'_i are 3-vector-valued parameters. For convenience, we work in the basis such that $\Delta_i = \Delta\delta_{i3}$. Furthermore, we collect the point-particle couplings involving Ψ as $W = W^\dagger := h' - \frac{i}{2}g'_i T_i$.

Upon quantization, the T_i can be identified with $\frac{i}{2}\sigma_i$, the generators of $\mathfrak{su}(2)$, and since they only live on the point-particle's world-line, it is easy to see that they are associated with a two-level nuclear state. Varying the action with respect to $y(\tau)$ (and neglecting the subdominant contribution from the W interactions), the nuclear dispersion relation

$$\langle N|\hat{p}_N^2 - M^2 + \Delta\sigma_z|N\rangle = 0, \tag{6.2}$$

($\hat{p}_N$ is the nuclear 4-momentum operator) leads to distinct nuclear states $|\uparrow\rangle$ with rest-frame energy $E_\uparrow = M + \Delta/2$ and $|\downarrow\rangle$ with rest-frame energy $E_\downarrow = M - \Delta/2$.

The bulk action for the system is exactly the single-particle Schrödinger action (2.1), and so the solutions for Ψ are precisely (2.7) and (2.8). However, the boundary condition (2.6) becomes:

$$\langle\uparrow\downarrow|4\pi\epsilon^2\partial_\epsilon\Psi|\Xi\rangle = \langle\uparrow\downarrow|W\Psi(\epsilon)|\Xi\rangle, \tag{6.3}$$

where $|\Xi\rangle$ is an appropriate Fock state, $|\uparrow\downarrow\rangle$ are the Fock states consisting of just the nucleus in the state with rest-frame energy $E_{\uparrow\downarrow}$, and Ψ is interpreted as an operator-valued field. Since energy can now be exchanged between the electron and the nucleus, the individual energies of the electron and the nucleus are no longer good quantum numbers, and a general single-electron Fock state must be a linear combination $|\Xi\rangle = |\Psi_\uparrow\rangle|\uparrow\rangle + |\Psi_\downarrow\rangle|\downarrow\rangle$, where $|\Psi_{\uparrow\downarrow}\rangle$ has energy $\omega_{\uparrow\downarrow}$ satisfying $\omega_\uparrow + \Delta/2 = \omega_\downarrow - \Delta/2$. Then in terms of the mode-functions $\Psi_{\uparrow\downarrow}(x) = e^{-i\omega_{\uparrow\downarrow}}\psi_{\uparrow\downarrow}$ (satisfying $\Psi|\Psi_{\uparrow\downarrow}\rangle = \Psi_{\uparrow\downarrow}(x)|\Psi_{\uparrow\downarrow}\rangle$), the boundary condition (6.3) is in components,

$$\begin{aligned} &4\pi\epsilon^2\partial_\epsilon\psi_\uparrow - W_{\uparrow\uparrow}\psi_\uparrow(\epsilon) - W_{\uparrow\downarrow}\psi_\downarrow(\epsilon) = 0 \qquad \text{and} \\ &4\pi\epsilon^2\partial_\epsilon\psi_\downarrow - W_{\downarrow\downarrow}\psi_\downarrow(\epsilon) - W_{\downarrow\uparrow}\psi_\uparrow(\epsilon) = 0, \end{aligned} \tag{6.4}$$

where we identified the T_i with $\frac{1}{2}\sigma_i$ so that $W = h'\mathbb{I}_{2\times2} + \frac{1}{4}g'_i\sigma_i$. The boundary condition (6.4) is now exactly the boundary condition (4.2) with $W \leftrightarrow \mathbf{h}$ and $\psi_{\uparrow\downarrow} \leftrightarrow \phi_{1,2}$.

Finally, defining $E := \omega_\uparrow + \Delta/2 = \omega_\downarrow - \Delta/2$, we observe $k_\uparrow^2 = 2m\omega_\uparrow = 2m(E - \Delta/2)$ and $k_\downarrow^2 = 2m\omega_\downarrow = 2m(E + \Delta/2)$. Choosing $\psi_\uparrow \leftrightarrow \psi_1$ and $\psi_\downarrow \leftrightarrow \psi_2$, we may then identify $k_1 = k_\uparrow$ and $k_2 = k_\downarrow$. At this point, a complete analogy with the two-species system is established, and the results are tabulated into a dictionary relating the two in **Table 1**. A true transfer reaction is one for which the final state involves both a different species of bulk particle *and* an altered state of the nucleus, so evidently would be equivalent to a model of 4 bulk species coupled to a single-state point-particle. As it stands however, this system is sufficient to describe, say, the low-energy behavior of a neutron that knocks a nucleus into its first excited state.

TABLE 1 | The dictionary that maps quantities in a two-bulk-species theory to quantities in a theory of a single bulk-species coupled to a point-particle with two accessible internal degrees of freedom.

Two-state nucleus		Two-species bulk
$\psi_\uparrow$, $\psi_\downarrow$	$\longleftrightarrow$	ψ_1, ψ_2
$k_\uparrow$, $k_\downarrow$	$\longleftrightarrow$	k_1, k_2
W	$\longleftrightarrow$	h

TABLE 2 | The dictionary that maps quantities in a unitary two-species theory to quantities in a non-unitary single-species theory.

Absorptive single-species		Unitary two-species
$\epsilon_\star$	$\longleftrightarrow$	ϵ_1
$\alpha_\star$	$\longleftrightarrow$	$n\pi - (2k_2\epsilon_3)^{\zeta_1}\left(\frac{\epsilon_3}{\epsilon_1}\right)^{\zeta_2}\frac{\lvert R\rvert}{y_1}\sin(\pi\zeta_2/2)\rvert$
$\hat{\lambda}_c$	$\longleftrightarrow$	$\hat{\lambda}_{11} - 4\frac{\lvert\hat{\lambda}_{12}\rvert^2}{[\hat{\lambda}_{22}+1]}$

7. SINGLE-PARTICLE SUBSECTOR

In many cases it is overkill to track all of the possible final state products of a particular interaction. This is especially the case in nuclear physics, where a summation over many unobserved final states is the basis of the highly successful optical model [14, 15]. The price one pays for the convenience of ignoring certain states is the loss of unitarity, and such a non-unitary point-particle EFT was the subject of Plestid et al. [13]. Here we can provide a very simple explicit example of how this non-unitarity can emerge in a subsector of a larger unitary theory. We achieve this correspondence by matching physical quantities, in a procedure that is significantly simpler than e.g., tracing the partition function over the states involving Ψ_2 [29, 30].

From Plestid et al. [13], the key to a point-particle inducing a violation of unitarity is allowing the point-particle coupling to be complex (h from section 2). In that case, the running of the coupling is the same as (2.9), except now the constant $-y \to e^{i\alpha_\star}$ is complex. That is:

$$\hat{\lambda}_c = \frac{1 - e^{i\alpha_\star}(\epsilon/\epsilon_\star)^{-\zeta}}{1 + e^{i\alpha_\star}(\epsilon/\epsilon_\star)^{-\zeta}}, \tag{7.1}$$

where $\hat{\lambda}_c$ is the now complex coupling. Similarly, the integration constant is analogous to (2.10),

$$\frac{C_-}{C_+} = (2ik\epsilon)^\zeta \frac{1 - \hat{\lambda}_c}{1 + \hat{\lambda}_c} = (2ik\epsilon_\star)^\zeta e^{i\alpha_\star}. \tag{7.2}$$

At this point, we essentially have everything we need. The ratio of integration constants $\frac{C_-}{C_+}$ is directly related to the physical quantities in the single-particle problem, so choosing to track either Ψ_1 or Ψ_2 tells us to equate (7.2) to C_{11} or C_{22} (respectively), and from that determine how the RG-invariants and couplings are related. The only obstruction at this point is that (4.15) would at face value suggest that $\alpha_\star = n\pi$ and there is no absorptive scattering. The error here is that inelastic scattering is a sub-leading effect[4], and to see it at the level of C_{11}, we would need to have computed that ratio of integration constants to sub-leading order in $k_i\epsilon$. This is not in itself a particularly challenging endeavor, and is done in the **Appendix B**. The result is that to sub-leading order, one finds (B.22) (choosing to track Ψ_1, tracking Ψ_2 follows trivially)

$$\begin{aligned} C_{11} &= -(2ik_1\epsilon)^{\zeta_1} \frac{\widehat{\mathcal{N}}_1}{\widehat{\mathcal{D}}} \left(1 - 4R \frac{\hat{\lambda}_{12}\hat{\lambda}_{21}}{\widehat{\mathcal{N}}_1 \widehat{\mathcal{D}}} (2ik_2\epsilon)^{\zeta_2}\right) \\ &= -y_1 (2ik_1\epsilon_1)^{\zeta_1}(1 + i\delta\alpha_1). \end{aligned} \tag{7.3}$$

From the last equality, we use that $\delta\alpha_1 \ll 1$ to define $e^{i\alpha_1} \approx -y_1(1 + i\delta\alpha_1)$ such that $\alpha_1 := n\pi + \delta\alpha_1$, with n an integer that satisfies $y_1 := -e^{in\pi}$. Since (7.3) is a perturbative expression, we may use the leading order (in $k_i\epsilon$) expressions for the couplings in $\delta\alpha_1$, and simply evaluate them at $\epsilon = \epsilon_1$. An alternative but more tedious approach would be to substitute the second equality in (7.3) into $\hat{\lambda}_{11}$ [taking the whole function to sub-leading order in $k_i\epsilon$ as in (C.12)] and solve for $\delta\alpha_1$ by demanding $\hat{\lambda}_{11}$ remain real at sub-leading order, as it must. No matter the approach, the result is

$$\delta\alpha_1 = -(2k_2\epsilon_3)^{\zeta_1} \left(\frac{\epsilon_3}{\epsilon_1}\right)^{\zeta_2} \frac{|R|}{y_1} \sin(\pi\zeta_2/2). \tag{7.4}$$

In this way, we have solved for the RG-invariant quantities (and so too the physical quantities) in the single-particle absorptive model in terms of the RG-invariants in the unitary two-species model simply by equating C_{11} to C_-/C_+. In fact, we can do even better than that. We can determine how the coupling $\hat{\lambda}_c$ relates to the various $\widehat{\lambda}_{ij}$ couplings. To do so, we simply arrange for $\widehat{\mathcal{N}}_A/\widehat{\mathcal{D}}$ to take the form of $(\hat{\lambda}_c - 1)/(\hat{\lambda}_c + 1)$.

$$\frac{\widehat{\mathcal{N}}_1}{\widehat{\mathcal{D}}} = \frac{4\left|\widehat{\lambda}_{12}\right|^2 - \left[\,\widehat{\lambda}_{11} - 1\right]\left[\,\widehat{\lambda}_{22} + 1\right]}{4\left|\widehat{\lambda}_{12}\right|^2 - \left[\,\widehat{\lambda}_{11} + 1\right]\left[\,\widehat{\lambda}_{22} + 1\right]} = \frac{\frac{\widehat{\lambda}_{11}[\,\widehat{\lambda}_{22}+1] - 4\left|\widehat{\lambda}_{12}\right|^2}{[\,\widehat{\lambda}_{22}+1]} - 1}{\frac{\widehat{\lambda}_{11}[\,\widehat{\lambda}_{22}+1] - 4\left|\widehat{\lambda}_{12}\right|^2}{[\,\widehat{\lambda}_{22}+1]} + 1}. \tag{7.5}$$

Evidently $\hat{\lambda}_c = \widehat{\lambda}_{11} - 4|\widehat{\lambda}_{12}|^2/[\widehat{\lambda}_{22} + 1]$. A check on this is to directly compute the combination $\widehat{\lambda}_{11} - 4|\widehat{\lambda}_{12}|^2/[\widehat{\lambda}_{22} + 1]$, in which case one finds it is exactly (7.1) with $\epsilon_\star$ and $\alpha_\star$ defined as above. This dictionary between these models is laid out in **Table 2**.

DATA AVAILABILITY STATEMENT

All datasets generated for this study are included in the article/supplementary material.

AUTHOR CONTRIBUTIONS

PH wrote most of the text and derived most of the results. CB provided significant guidance, corrected errors, helped with interpretations, and provided feedback on the manuscript.

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[4]The way to see this is through the catalysis cross-section (5.15). Absorptive scattering generically scales as a/k for some absorptive scattering length a. The derived cross-section (5.15) identifies $a \sim (k_2\epsilon_3)\epsilon_3$ and so is generically a subdominant effect in the point-particle EFT regime.

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Conflict of Interest: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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APPENDIX

A. MULTI-PARTICLE PARTIAL-WAVE SCATTERING

Here we review the general framework of partial-wave scattering, including discussion of inelastic and multi-channel scattering.

A.1. Single Particle Elastic Scattering

We consider a spinless particle scattering off of a spinless, infinitely massive object at rest at the origin, through a spherically symmetric interaction $V(r)$. As usual, we employ the ansatz that at large distances from the target, the wavefunction of the incident particle is the sum of a plane wave incident along the z-axis and a scattered spherical wave:

$$\psi_{\infty}^{\text{Ans}}(r) \to \mathcal{C}\left(e^{ikz} + f(\theta,\phi)\frac{e^{ikr}}{r}\right). \tag{A1}$$

The differential cross-section is the ratio of the flux of the scattered particles F_{sc} to the flux of the incoming particles F_{in}. With an incident beam of N particles, the incoming flux is $N\,\mathbf{j}_{in}\cdot\mathbf{e}_z = N\,|\mathcal{C}|^2\,k/m$, and the scattered flux is $N|\mathcal{C}|^2\left|f(\theta,\phi)\right|^2 k/mr^2$, so that and is given by

$$\frac{d\sigma}{d\Omega} := \frac{F_{sc}}{F_{in}} = \frac{1}{F_{in}}\,\mathbf{j}_{sc}\cdot\mathbf{e}_r\,r^2 = |f(\theta)|^2. \tag{A2}$$

And for a spherically symmetric scatterer, $f(\theta,\phi) = f(\theta)$.

At the same time, we consider solutions to the full Schrodinger equation

$$\frac{1}{r^2}\partial_r\left(r^2\partial_r\psi(r)\right) - \left[\frac{\ell(\ell+1)}{r^2} + 2mV(r) - k^2\right]\psi(r) = 0, \tag{A3}$$

with $k^2 := 2mE$, and the full wavefunction expanded in a series of spherical harmonics $\Psi(\vec{x},t) = e^{-iEt}\psi(r)Y_{\ell 0}$ (where we set $m = 0$ due to conservation of angular momentum). The asymptotic form of these radial functions is:

$$\psi_{\infty}^{\text{Sch}}(r) \to A_\ell\frac{e^{i(kr-\ell\pi/2)}}{2ikr} + B_\ell\frac{e^{-i(kr-\ell\pi/2)}}{2ikr}, \tag{A4}$$

Finding $f(\theta)$ now amounts to matching (A1) and (A4). This can be accomplished by writing the plane-wave e^{ikz} in terms of Legendre polynomials. The standard expansion is given as Landau and Lifshitz [31]

$$\begin{aligned} e^{ikz} &= \sum_{\ell=0}^{\infty}(2\ell+1)i^\ell j_\ell(kr)P_\ell(\cos(\theta)) \\ &\to \sum_{\ell=0}^{\infty}(2\ell+1)i^\ell\frac{e^{i(kr-\ell\pi/2)} - e^{-i(kr-\ell\pi/2)}}{2ikr}P_\ell(\cos(\theta)). \end{aligned} \tag{A5}$$

Choosing the Condon-Shortly phase convention, the spherical harmonics can be written $Y_\ell^0 = \sqrt{(2\ell+1)/4\pi}\,P_\ell(\cos(\theta))$, so by computing the difference:

$$\psi_{\infty}^{\text{Sch}}(r) - \mathcal{C}e^{ikz} = \mathcal{C}f(\theta)\frac{e^{ikr}}{r}, \tag{A6}$$

one finds first:

$$B_\ell = -\sqrt{4\pi(2\ell+1)}\,i^\ell\mathcal{C}, \tag{A7}$$

set by the fact that there can be no incoming wave in the scattered wavefunction. Finally, one finds

$$f(\theta) = \frac{1}{2ik}\sum_{\ell=0}^{\infty}(2\ell+1)[S_\ell - 1]P_\ell(\theta), \tag{A8}$$

Where $S_\ell = -A_\ell/B_\ell$ is the scattering matrix element. When the scattering is elastic as we've just described ($k_{\text{out}} = k_{\text{in}}$), the matrix element $S_\ell = e^{2i\delta_\ell}$ is a pure phase. Otherwise, when the scattering is inelastic and probability is lost, S_ℓ is just a complex number, but it is still common [14] to parameterize it as $S_\ell^{(in)} = e^{2i\gamma_\ell}$, where γ_ℓ is now a complex number.

Finally, the total cross-section is computed as the integral over the differential cross-section, which is (using the orthogonality of the Legendre polynomials)

$$\sigma = \int d\Omega\frac{d\sigma}{d\Omega} = \frac{\pi}{k^2}\sum_\ell(2\ell+1)|S_\ell - 1|^2. \tag{A9}$$

A.2. Multi-Channel Scattering

It is a simple matter to generalize the above to multi-channel scattering. We treat the case of two species of particles, but as detailed in section 6 the results are more general. Without loss of generality, we will only look at $1 \to X$ scattering.

Following Landau and Lifshitz [27], we begin by assuming the asymptotic forms for each species:

$$\psi_1^{\text{Ans}}(r\to\infty) \to \mathcal{C}\left(e^{ik_1 z} + f_1(\theta,\phi)\frac{e^{ik_1 r}}{r}\right). \tag{A10}$$

and

$$\psi_2^{\text{Ans}}(r\to\infty) \to \mathcal{C}f_2(\theta,\phi)\frac{e^{ik_2 r}}{r}. \tag{A11}$$

The differential cross-sections are defined in exactly the same way as the above. This means the $1 \to 1$ scattering is exactly given by (A9), while for $1 \to 2$ scattering we have

$$\frac{d\sigma^{1\to 2}}{d\Omega} = \frac{k_2}{k_1}\frac{m_1}{m_2}|f_2(\theta)|^2. \tag{A12}$$

Particle 2 satisfies the same Schrödinger equation (A3), and so has the same asymptotic form (A4). Matching to the ansatz is then as simple as

$$\psi_{2,\infty}^{\text{Sch}} = \mathcal{C}f_2(\theta)\frac{e^{ik_2 r}}{r}, \tag{A13}$$

which produces

$$B_{2\ell} = 0, \tag{A14}$$

and

$$\begin{aligned} f_2(\theta) &= \frac{1}{2ik_2\mathcal{C}} \sum_\ell e^{-i\pi\ell/2} A_{2\ell} Y^0_\ell(\theta) \\ &= \frac{1}{2ik_2} \sum_\ell (2\ell+1) S^{(\ell)}_{12} P_\ell(\cos\theta), \end{aligned} \tag{A15}$$

which defines the scattering matrix element $S^{(\ell)}_{12} = e^{-i\pi\ell/2}[4\pi(2\ell+1)]^{-1/2}A_{2\ell}/\mathcal{C}$. Finally, the total cross-section is

$$\sigma^{1\to 2} = \frac{\pi}{k_1 k_2}\frac{m_1}{m_2}\sum_\ell (2\ell+1)|S^{(\ell)}_{12}|^2. \tag{A16}$$

One important observation: as long as $S^{(\ell)}_{12} \neq 0$ for any ℓ, then $S^{(\ell)}_{11} = e^{2i\gamma^{(\ell)}_{11}}$ must satisfy that the phase $\gamma^{(\ell)}_{11}$ is complex, since some of the probability flux of the incident particle 1 must have transferred to particle 2.

B. SOLVING FOR 2-PARTICLE INTEGRATION CONSTANT RATIOS

Here we outline the details of the main calculation in section 4.1. We do this for $1 \to X$ scattering, but the results are easily applied to $2 \to X$ scattering by inverting $1 \leftrightarrow 2$.

We begin with the boundary condition (4.2), and the general forms

$$\psi_i = C_{i+}\psi_{i+} + C_{i-}\psi_{i-}, \tag{A17}$$

where $i = 1, 2$. For $1 \to X$ scattering, we use $C_{2+} = R\,C_{2-}$ with R defined in (4.4), and the boundary conditions are:

$$\widehat{\psi}'_{1+} + C_{11}\widehat{\psi}'_{1-} = h_{11}(\psi_{1+} + C_{11}\psi_{1-}) + h_{12}C_{12}(\psi_{2+}R + \psi_{2-}), \quad \text{and} \tag{A18a}$$

$$C_{12}(\widehat{\psi}'_{2+}R + \widehat{\psi}'_{2-}) = h_{22}C_{12}(\psi_{2+}R_2 + \psi_{2-}) + h_{21}(\psi_{1+} + C_{11}\psi_{1-}). \tag{A18b}$$

where we define $\widehat{\psi}'_{i\pm} := \frac{2\pi\epsilon^2}{m_i}\partial_\epsilon\psi_{i\pm}$, and as in (4.3), we define $C_{11} := C_{1-}/C_{1+}$ and $C_{12} := C_{2-}/C_{1+}$.

Rearranging (A18a) for C_{12}, one finds

$$C_{12} = \frac{\left[\widehat{\psi}'_{1+} - h_{11}\psi_{1+}\right] + C_{11}\left[\widehat{\psi}'_{1-} - h_{11}\psi_{1-}\right]}{h_{12}[\psi_{2+}R + \psi_{2-}]}. \tag{A19}$$

Substituting in (A18b),

$$\begin{aligned} &\left\{[\widehat{\psi}'_{1+} - h_{11}\psi_{1+}] + C_{11}[\widehat{\psi}'_{1-} - h_{11}\psi_{1-}]\right\} \\ &Z = |h_{12}|^2[\psi_{1+} + C_{11}\psi_{1-}], \end{aligned} \tag{A20}$$

where

$$Z := \frac{\widehat{\psi}'_{2+}R + \widehat{\psi}'_{2-}}{\psi_{2+}R + \psi_{2-}} - h_{22}. \tag{A21}$$

Finally rearranging, we have

$$C_{11} = -\frac{\psi_{1+}}{\psi_{1-}}\frac{\left[|h_{12}|^2 - \left[\frac{\widehat{\psi}'_{1+}}{\psi_{1+}} - h_{11}\right]Z\right]}{\left[|h_{12}|^2 - \left[\frac{\widehat{\psi}'_{1-}}{\psi_{1-}} - h_{11}\right]Z\right]} \tag{A22}$$

Plugging this back into (A19), we have

$$\begin{aligned} C_{12} &= \frac{\psi_{1+}}{\psi_{2-}}\frac{\left[\frac{\widehat{\psi}'_{1+}}{\psi_{1+}} - h_{11}\right]\left[|h_{12}|^2 - \left[\frac{\widehat{\psi}'_{1-}}{\psi_{1-}} - h_{11}\right]Z\right] - [+ \leftrightarrow -]}{h_{12}\left[R\frac{\psi_{2+}}{\psi_{2-}} + 1\right]\left[|h_{12}|^2 - \left[\frac{\widehat{\psi}'_{1-}}{\psi_{1-}} - h_{11}\right]Z\right]}, \\ &= \frac{\psi_{1+}}{\psi_{2-}}\frac{\left[\frac{\widehat{\psi}'_{1+}}{\psi_{1+}} - \frac{\widehat{\psi}'_{1-}}{\psi_{1-}}\right]h_{21}}{\left[R\frac{\psi_{2+}}{\psi_{2-}} + 1\right]\left[|h_{12}|^2 - \left[\frac{\widehat{\psi}'_{1-}}{\psi_{1-}} - h_{11}\right]Z\right]}. \end{aligned} \tag{A23}$$

The integration constants in the $2 \to X$ system are solved for in the same way. Solutions for $C_{22} = C_{2-}/C_{2+}$ and $C_{21} = C_{1-}/C_{2+}$ in the $2 \to X$ are obtained directly from (A22) and (A23) (respectively) by simply inverting $1 \leftrightarrow 2$.

In order to make use of these formulae, we now have to take the small-r limit of the mode functions to the appropriate order.

B.1. Leading-Order in $k_i\epsilon$

First, we make the usual leading-order approximation. For ψ_1, this is exactly as in (4.6):

$$\begin{aligned} \psi_1(\epsilon) &\approx x_1^{-1/2}\left[C_{1+}x_1^{\zeta_1/2} + C_{1-}x_1^{-\zeta_1/2}\right], \quad \text{and} \\ \partial_r\psi_1(\epsilon) &\approx ik_1x_1^{-3/2}\left[(\zeta_1-1)C_{1+}x_1^{\zeta_1/2} - (\zeta_1+1)C_{1-}x_1^{-\zeta_1/2}\right], \end{aligned} \tag{A24}$$

where for convenience here we define $x_i := (2ik_i\epsilon)$, for $i = 1, 2$. Here we keep both the divergent $(-)$ and the (often) finite $(+)$ term because the ratio C_{1-}/C_{1+} arises from the point-particle dynamics, and so is of the order $k_i\epsilon \ll 1$, which allows the two terms in (A24) to compete. For particle 2 however, this is not the case. $C_{2+} = R\,C_{2-}$ with $R \sim \mathcal{O}(1)$ so that there is no balancing of the modes, and the divergent mode is simply dominant. That is:

$$\begin{aligned} \psi_2(\epsilon) &\approx C_{2-}x_2^{-1/2-\zeta_2/2}, \quad \text{and} \\ \partial_r\psi_2(\epsilon) &\approx -(\zeta_2+1)ik_2C_{2-}x_2^{-3/2-\zeta_2/2}. \end{aligned} \tag{A25}$$

With these approximations, we compute:

$$\begin{aligned} &\frac{\widehat{\psi}'_{i\pm}}{\psi_{i\pm}} \approx -\frac{\pi\epsilon}{m_i}(1 \mp \zeta_i), \\ &\frac{\psi_{1+}}{\psi_{1-}} \approx (2ik_1\epsilon)^{\zeta_1}, \\ &\frac{\psi_{2+}}{\psi_{2-}} \approx 0, \quad \text{and} \\ &Z \approx \frac{\widehat{\psi}'_{2-}}{\psi_{2-}} - h_{22} \approx -\left[(1+\zeta_2)\frac{\pi\epsilon}{m_2} + h_{22}\right]. \end{aligned} \tag{A26}$$

Then to leading order in $k_i\epsilon$, it is found that:

$$C_{11} \approx -(2ik_1\epsilon)^{\zeta_1} \frac{\left[|h_{12}|^2 - \left[\frac{\pi\epsilon}{m_1}(1-\zeta_1)+h_{11}\right]\left[(1+\zeta_2)\frac{\pi\epsilon}{m_2}+h_{22}\right]\right]}{\left[|h_{12}|^2 - \left[\frac{\pi\epsilon}{m_1}(1+\zeta_1)+h_{11}\right]\left[(1+\zeta_2)\frac{\pi\epsilon}{m_2}+h_{22}\right]\right]}, \tag{A27}$$

and

$$C_{12} = (2ik_1\epsilon)^{\zeta_1/2}(2ik_2\epsilon)^{\zeta_2/2}\sqrt{\frac{k_2}{k_1}} \frac{2\pi\epsilon\zeta_1 h_{21}}{m_1\left[|h_{12}|^2 - \left[\frac{\pi\epsilon}{m_1}(1+\zeta_1)+h_{11}\right]\left[(1+\zeta_2)\frac{\pi\epsilon}{m_2}+h_{22}\right]\right]} \tag{A28}$$

It will become apparent that a redefinition of parameters can significantly clean up our equations. Drawing from the next appendix, we define

$$\begin{aligned} \hat{\lambda}_{11} &:= \frac{1}{\zeta_1}\left(\frac{m_1 h_{11}}{\pi\epsilon}+1\right) \qquad \hat{\lambda}_{12} := \frac{h_{12}\sqrt{m_1 m_2}}{2\pi\epsilon\sqrt{\zeta_1\zeta_2}}, \\ \hat{\lambda}_{22} &:= \frac{1}{\zeta_2}\left(\frac{m_2 h_{22}}{\pi\epsilon}+1\right) \qquad \hat{\lambda}_{21} := \frac{h_{21}\sqrt{m_1 m_2}}{2\pi\epsilon\sqrt{\zeta_1\zeta_2}}. \end{aligned} \tag{A29}$$

In terms of these new variables, the integration constants read:

$$C_{11} = -(2ik_1\epsilon)^{\zeta_1}\frac{\left[4\hat{\lambda}_{12}\hat{\lambda}_{21} - \left[\hat{\lambda}_{11}-1\right]\left[\hat{\lambda}_{22}+1\right]\right]}{\left[4\hat{\lambda}_{12}\hat{\lambda}_{21} - \left[\hat{\lambda}_{11}+1\right]\left[\hat{\lambda}_{22}+1\right]\right]}, \tag{A30}$$

and

$$C_{12} = (2ik_1\epsilon)^{\zeta_1/2}(2ik_2\epsilon)^{\zeta_2/2}\sqrt{\frac{m_2 k_2\zeta_1}{m_1 k_1\zeta_2}} \frac{4\hat{\lambda}_{21}}{\left[4\hat{\lambda}_{12}\hat{\lambda}_{21} - \left[\hat{\lambda}_{11}+1\right]\left[\hat{\lambda}_{22}+1\right]\right]}. \tag{A31}$$

B.2. Sub-Leading-Order in $k_i\epsilon$

To leading order, $C_{11} \sim (2ik\epsilon)^{\zeta_1}$, so that to leading order $S_{11}^{(\ell)}$ is a pure phase. In order to see the emergence of an absorptive single-particle model in the particle 1 subsector of the theory (as covered in section 7), it is necessary to compute C_{11} to the next order in $k_i\epsilon$. To that end, recall:

$$\psi_\pm = (2ik\epsilon)^{\frac{1}{2}(-1\pm\zeta)}e^{-ik\epsilon}\mathcal{M}\left[\frac{1}{2}(1\pm\zeta), 1\pm\zeta, 2ik\epsilon\right], \tag{A32}$$

so that

$$\begin{aligned} \psi_\pm &\approx (2ik\epsilon)^{\frac{1}{2}(-1\pm\zeta)}\left[1 - ik\epsilon + \mathcal{O}\left((k\epsilon)^2\right)\right]\left[1 + ik\epsilon + \mathcal{O}\left((k\epsilon)^2\right)\right], \\ &\approx (2ik\epsilon)^{\frac{1}{2}(-1\pm\zeta)}\left[1 + \mathcal{O}\left((k\epsilon)^2\right)\right] \end{aligned} \tag{A33}$$

so at least for $\zeta < 2$, the leading correction is only in ψ_2, and is to include the $(+)$ mode, since it is only a factor of $(k_2\epsilon)^{\zeta_2}$ compared to the two powers from all other higher-order corrections. In fact this is a property only of systems without a $1/r$ potential, as in that case the leading correction from the hypergeometric factor does not cancel that from the exponential.

Pushing through then, we repeat the calculation from the previous section, now using

$$\begin{aligned} \psi_2(\epsilon) &\approx C_{2-}x_2^{-1/2}\left[x_2^{-\zeta_2/2} + R\,x_2^{\zeta_2/2}\right], \quad \text{and} \\ \partial_r\psi_2(\epsilon) &\approx ik_2 C_{2-}x_2^{-3/2}\left[-(\zeta_2+1)x_2^{-\zeta_2/2} + (\zeta_2-1)R\,x_2^{\zeta_2/2}\right]. \end{aligned} \tag{A34}$$

With these approximations, we compute:

$$\begin{aligned} \frac{\hat{\psi}'_{i\pm}}{\psi_{i\pm}} &\approx -\frac{\pi\epsilon}{m_i}(1\mp\zeta_i), \\ \frac{\psi_{i+}}{\psi_{i-}} &\approx (2ik_i\epsilon)^{\zeta_i}, \quad \text{and} \\ Z &\approx \frac{\hat{\psi}'_{2-}+R\,\hat{\psi}'_{2+}}{\psi_{2-}+R\,\psi_{2+}} - h_{22} = \frac{\hat{\psi}'_{2-}}{\psi_{2-}}\frac{1+R\,\hat{\psi}'_{2+}/\hat{\psi}'_{2-}}{1+R\,\psi_{2+}/\psi_{2-}} - h_{22} \\ &\approx -\left[(1+\zeta_2)\frac{\pi\epsilon}{m_2}\right]\left\{1 + R\left(\frac{\hat{\psi}'_{2+}}{\hat{\psi}'_{2-}} - \frac{\psi_{2+}}{\psi_{2-}}\right)\right\} - h_{22}, \\ &= -\left[(1+\zeta_2)\frac{\pi\epsilon}{m_2}\right]\left\{1 - \frac{2\zeta_2 R}{\zeta_2+1}(2ik_2\epsilon)^{\zeta_2}\right\} - h_{22}. \end{aligned} \tag{A35}$$

Substituting in (A22), one finds

$$\begin{aligned} C_{1-} &\approx -(2ik_1\epsilon)^{\zeta_1}\frac{\left\{\begin{array}{c} |h_{12}|^2 - \left[\frac{\pi\epsilon}{m_1}(1-\zeta_1)+h_{11}\right] \\ \left[(1+\zeta_2)\frac{\pi\epsilon}{m_2}\left(1-\frac{2\zeta_2 R}{\zeta_2+1}(2ik_2\epsilon)^{\zeta_2}\right)+h_{22}\right] \end{array}\right\}}{\left\{\begin{array}{c} |h_{12}|^2 - \left[\frac{\pi\epsilon}{m_1}(1+\zeta_1)+h_{11}\right] \\ \left[(1+\zeta_2)\frac{\pi\epsilon}{m_2}\left(1-\frac{2\zeta_2 R}{\zeta_2+1}(2ik_2\epsilon)^{\zeta_2}\right)+h_{22}\right] \end{array}\right\}}, \\ &= -(2ik_1\epsilon)^{\zeta_1}\frac{\mathcal{N}_1 + \left[\frac{\pi\epsilon}{m_1}(1-\zeta_1)+h_{11}\right]\frac{2\pi\epsilon\zeta_2 R}{m_2}(2ik_2\epsilon)^{\zeta_2}}{\mathcal{D} + \left[\frac{\pi\epsilon}{m_1}(1+\zeta_1)+h_{11}\right]\frac{2\pi\epsilon\zeta_2 R}{m_2}(2ik_2\epsilon)^{\zeta_2}}, \\ &\approx -(2ik_1\epsilon)^{\zeta_1}\frac{\mathcal{N}_1}{\mathcal{D}}\left\{\begin{array}{c} 1 + \left[\begin{array}{c} \frac{\left[\frac{\pi\epsilon}{m_1}(1-\zeta_1)+h_{11}\right]}{\mathcal{N}_1} \\ -\frac{\left[\frac{\pi\epsilon}{m_1}(1+\zeta_1)+h_{11}\right]}{\mathcal{D}} \end{array}\right] \end{array}\right\}\frac{2\pi\epsilon\zeta_2 R}{m_2}(2ik_2\epsilon)^{\zeta_2}, \end{aligned} \tag{A36}$$

where

$$\begin{aligned} \mathcal{N}_1 &:= |h_{12}|^2 - \left[\frac{\pi\epsilon}{m_1}(1-\zeta_1)+h_{11}\right]\left[(1+\zeta_2)\frac{\pi\epsilon}{m_2}+h_{22}\right], \quad \text{and} \\ \mathcal{D} &:= |h_{12}|^2 - \left[\frac{\pi\epsilon}{m_1}(1+\zeta_1)+h_{11}\right]\left[(1+\zeta_2)\frac{\pi\epsilon}{m_2}+h_{22}\right]. \end{aligned} \tag{A37}$$

Then (A36) simplifies to:

$$C_{11} = -(2ik_1\epsilon)^{\zeta_1}\frac{\widehat{\mathcal{N}}_1}{\widehat{\mathcal{D}}}\left\{1 - 4R\,\frac{\hat{\lambda}_{12}\hat{\lambda}_{21}}{\widehat{\mathcal{N}}_1\widehat{\mathcal{D}}}(2ik_2\epsilon)^{\zeta_2}\right\}. \tag{A38}$$

C. SOLVING FOR POINT-PARTICLE COUPLINGS

To find the running of the point-particle couplings, we need to isolate for them in the boundary conditions. To do so, we follow the same prescription as B. Write:

$$\psi_i = C_{i+}\psi_{i+} + C_{i-}\psi_{i-}, \tag{A39}$$

where $i = 1, 2$. We again use (5.8) to define $C_{11} := C_{1-}/C_{1+}$ and $C_{12} := C_{2-}/C_{1+}$ in the $1 \to X$ system, and analogously $C_{22} := C_{2-}/C_{2+}$ and $C_{21} := C_{1-}/C_{2+}$ in the $2 \to X$ system.

For convenience, define the following:

$$\psi_{11} := \psi_{1+} + C_{11}\psi_{1-} \qquad \text{and} \qquad \psi_{12} := C_{12}\left[R\psi_{2+} + \psi_{2-}\right] \tag{A40}$$

for the $1 \to X$ system, and

$$\psi_{22} := \psi_{2+} + C_{22}\psi_{2-} \qquad \text{and} \qquad \psi_{21} := C_{21}\left[R\psi_{1+} + \psi_{1-}\right] \tag{A41}$$

for the $2 \to X$ system. The small-r boundary conditions (4.5) and (4.10) can be written

$$\hat{\psi}'_{11} = h_{11}\psi_{11} + h_{12}\psi_{12}, \quad \text{and} \tag{A42}$$

$$\hat{\psi}'_{12} = h_{22}\psi_{12} + h_{21}\psi_{11}, \tag{A43}$$

and

$$\hat{\psi}'_{21} = h_{11}\psi_{21} + h_{12}\psi_{22}, \quad \text{and} \tag{A44}$$

$$\hat{\psi}'_{22} = h_{22}\psi_{22} + h_{21}\psi_{21}, \tag{A45}$$

As in **Appendix B**, we define $\hat{\psi}' := 4\pi\epsilon^2\partial_\epsilon\psi$. Using (A42) and (A44), we can isolate for h_{11} and h_{12}:

$$h_{11} = \frac{\hat{\psi}'_{11}\psi_{22} - \hat{\psi}'_{21}\psi_{12}}{\psi_{11}\psi_{22} - \psi_{21}\psi_{12}} \qquad \text{and} \qquad h_{12} = \frac{\hat{\psi}'_{11}\psi_{21} - \hat{\psi}'_{21}\psi_{11}}{\psi_{12}\psi_{21} - \psi_{22}\psi_{11}}. \tag{A46}$$

Similarly, using (A43) and (A45), we can isolate for h_{22} and h_{21}:

$$h_{22} = \frac{\hat{\psi}'_{12}\psi_{21} - \hat{\psi}'_{22}\psi_{11}}{\psi_{12}\psi_{21} - \psi_{22}\psi_{11}} \qquad \text{and} \qquad h_{21} = \frac{\hat{\psi}'_{12}\psi_{22} - \hat{\psi}'_{22}\psi_{12}}{\psi_{11}\psi_{22} - \psi_{21}\psi_{12}}. \tag{A47}$$

To make use of these formulae, we approximate ψ_{ij} using the small-r forms as used in **Appendix B**:

$$\psi_{11(22)}(\epsilon) \approx x_{1(2)}^{-1/2}\left[x_{1(2)}^{\zeta_{1(2)}/2} + C_{11(22)}x_{1(2)}^{-\zeta_{1(2)}/2}\right], \quad \text{and}$$

$$4\pi\epsilon^2\partial_r|_\epsilon\psi_{11(22)}(\epsilon) \approx 2\pi\epsilon\, x_{1(2)}^{-1/2}\begin{bmatrix}(\zeta_{1(2)}-1)x_{1(2)}^{\zeta_{1(2)}/2} \\ -(\zeta_{1(2)}+1)C_{11(22)}x_{1(2)}^{-\zeta_{1(2)}/2}\end{bmatrix}, \tag{A48}$$

and

$$\psi_{21(12)}(\epsilon) \approx C_{21(12)}x_{1(2)}^{-1/2-\zeta_{1(2)}/2}, \quad \text{and}$$

$$4\pi\epsilon^2\partial_r|_\epsilon\psi_{21(12)}(\epsilon) \approx -(\zeta_{1(2)}+1)2\pi\epsilon\, C_{21(12)}x_{1(2)}^{-1/2-\zeta_{1(2)}/2}. \tag{A49}$$

where again, $x_i := (2ik_i\epsilon)$, with $i = 1, 2$. Substituting (A48) and (A49) into (A46) and (A47), we have the following. For h_{11} we find

$$\begin{aligned}\hat{\lambda}_{11} &= \frac{\begin{matrix}(x_1^{\zeta_1/2} - C_{11}x_1^{-\zeta_2/2})(x_2^{\zeta_1/2} + C_{22}x_2^{-\zeta_2/2}) \\ +C_{21}C_{12}x_1^{-\zeta_1/2}x_2^{-\zeta_2/2}\end{matrix}}{\begin{matrix}(x_1^{\zeta_1/2} + C_{11}x_1^{-\zeta_2/2})(x_2^{\zeta_1/2} + C_{22}x_2^{-\zeta_2/2}) \\ -C_{21}C_{12}x_1^{-\zeta_1/2}x_2^{-\zeta_2/2}\end{matrix}}, \\ &= \frac{(1 - C_{11}x_1^{-\zeta_1})(1 + C_{22}x_2^{-\zeta_2}) + C_{21}C_{12}x_1^{-\zeta_1}x_2^{-\zeta_2}}{(1 + C_{11}x_1^{-\zeta_1})(1 + C_{22}x_2^{-\zeta_2}) - C_{21}C_{12}x_1^{-\zeta_1}x_2^{-\zeta_2}},\end{aligned} \tag{A50}$$

which defines $\hat{\lambda}_{11} := \frac{1}{\zeta_1}\left(\frac{m_1 h_{11}}{\pi\epsilon} + 1\right)$. Notice the limit $C_{21} = C_{12} \to 0$ reduces $\hat{\lambda}_{11}$ to the single-species running (2.9), as it should (the limit in which there is no mixing between particle species). For h_{12}, we have

$$\begin{aligned}\hat{\lambda}_{12} &= \sqrt{\frac{m_2\zeta_1}{m_1\zeta_2}}\frac{C_{21}\left(\frac{x_1}{x_2}\right)^{-1/2}}{\begin{matrix}(x_1^{\zeta_1/2} + C_{11}x_1^{-\zeta_2/2})(x_2^{\zeta_1/2} + C_{22}x_2^{-\zeta_2/2}) \\ -C_{21}C_{12}x_1^{-\zeta_1/2}x_2^{-\zeta_2/2}\end{matrix}}, \\ &= \sqrt{\frac{m_2\zeta_1}{m_1\zeta_2}}\frac{C_{21}\left(\frac{x_1}{x_2}\right)^{-1/2}x_1^{-\zeta_1/2}x_2^{-\zeta_2/2}}{(1 + C_{11}x_1^{-\zeta_1})(1 + C_{22}x_2^{-\zeta_2}) - C_{21}C_{12}x_1^{-\zeta_1}x_2^{-\zeta_2}},\end{aligned} \tag{A51}$$

with now $\hat{\lambda}_{12} := \frac{h_{12}\sqrt{m_1 m_2}}{2\pi\epsilon\sqrt{\zeta_1\zeta_2}}$. Notice again the clean limit $h_{12} \to 0$ when $C_{21} \to 0$. The rest follow easily:

$$\hat{\lambda}_{21} = \sqrt{\frac{m_1\zeta_2}{m_2\zeta_1}}\frac{C_{12}\left(\frac{x_2}{x_1}\right)^{-1/2}x_1^{-\zeta_1/2}x_2^{-\zeta_2/2}}{(1 + C_{11}x_1^{-\zeta_1})(1 + C_{22}x_2^{-\zeta_2}) - C_{21}C_{12}x_1^{-\zeta_1}x_2^{-\zeta_2}}, \tag{A52}$$

similarly with $\hat{\lambda}_{21} := \frac{h_{21}\sqrt{m_1 m_2}}{2\pi\epsilon\sqrt{\zeta_1\zeta_2}}$. Lastly,

$$\hat{\lambda}_{22} = \frac{(1 + C_{11}x_1^{-\zeta_1})(1 - C_{22}x_2^{-\zeta_2}) + C_{21}C_{12}x_1^{-\zeta_1}x_2^{-\zeta_2}}{(1 + C_{11}x_1^{-\zeta_1})(1 + C_{22}x_2^{-\zeta_2}) - C_{21}C_{12}x_1^{-\zeta_1}x_2^{-\zeta_2}}, \tag{A53}$$

with $\hat{\lambda}_{22} := \frac{1}{\zeta_2}\left(\frac{m_2 h_{22}}{2\pi\epsilon} + 1\right)$.

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Self-Adjoint Extension Approach for Singular Hamiltonians in (2 + 1) Dimensions

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In this work, we review two methods used to approach singular Hamiltonians in (2 + 1) dimensions. Both methods are based on the self-adjoint extension approach. It is very common to find singular Hamiltonians in quantum mechanics, especially in quantum systems in the presence of topological defects, which are usually modeled by point interactions. In general, it is possible to apply some kind of regularization procedure, as the vanishing of the wave function at the location of the singularity, ensuring that the wave function is square-integrable and then can be associated with a physical state. However, a study based on the self-adjoint extension approach can lead to more general boundary conditions that still gives acceptable physical states. We exemplify the methods by exploring the bound and scattering scenarios of a spin 1/2 charged particle with an anomalous magnetic moment in the Aharonov-Bohm potential in the conical space.

Keywords: curved space, self-adjoint operator, scattering, bound state, singular Hamiltonian operator, spin, anomalous magnetic moment

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1. INTRODUCTION

Singular and pathological Hamiltonians are quite common in quantum mechanics and already have a long history [1]. Probably, the first work to deal with δ-like singularities was in the Kronig-Penny model [2] for the description of the band energy in solid-state physics. Since then, point interactions have been of great interest in various branches of physics for their relevance as solvable models [3]. For instance, in the famous Aharonov-Bohm (AB) effect [4] of spin-1/2 particles [5–7] a two-dimensional δ function appears as the mathematical description of the Zeeman interaction between the spin and the magnetic flux tube [8, 9]. The presence of this δ function cannot be discarded when the electron spin is taken into account and it leads to changes in the scattering amplitude and cross-section [6]. This question can also be understood in connection with the quantum mechanics of a particle in a δ function potential in one dimension. When we wish to solve the problem for bound states, it is well-known that such a function guarantees at least one bound state [10, 11], and this property is maintained when studying the quantum mechanics of other physical systems in the presence of external magnetic fields. The inclusion of the spin element in the approach of the AB problem allows us to establish an exact equivalence with another well-known effect in the literature, namely the Aharonov-Casher (AC) effect [12]. In the AC effect, a spin-1/2 neutral particle with a magnetic moment is placed in an electric field generated by an infinitely long, an infinitesimally thin line of charge. The interaction term involving the particle spin with the electric field in the AC Hamiltonian is proportional to the δ function. Some works in the literature state that point

interaction does not affect the scattering cross-section [13]. However, as in the spin-1/2 particle AB problem, the solution of the equation of motion via the self-adjoint extension in the spin-1/2 neutral particle AC problem reveals that the presence of the δ function changes the scattering phase shift and consequently the S-matrix [14, 15].

The study of physical systems with singular Hamiltonians appears in various contexts of physics. In reference [16], the discrete spectrum of a massive particle trapped in an infinitely long cylinder with two attractive delta-interactions in the cosmic string spacetime is studied. The authors showed that the physical effects due to the cosmic string background are similar to those of the AB effect in quantum mechanics. This is verified when the cosmic string determines a deviation on the trajectory of a particle, despite the locally flat character of the manifold. In reference [17], the one-dimensional spinless Salpeter Hamiltonian with finitely many Dirac delta potentials was solved using the heat kernel techniques and self-adjoint extension method. As in the case involving a single δ potential, the model requires a renormalization to be made. They investigated the problem in the context of bound states and showed that the ground state energy is bounded from below. Besides, they also showed that there exists a unique self-adjoint operator associated with the resolvent formula and obtained an explicit wave function formula for N centers. The approach using this model to the scattering problem was addressed in reference [18]. Such a model is a generalization of the work in reference [19], where the Schrödinger equation for a relativistic point particle in an external one-dimensional δ-function potential was studied using dimensional regularization.

The physical regularization used in these models is consistent with the self-adjoint extension theory and the idea can also be used to study other versions of the Kronig-Penney model in condensed matter physics. Different forms of Kronig-Penney-type Hamiltonians can be found in the literature [20, 21]. To approach singular Hamiltonian, it is more convenient to apply von Neumann's theory of self-adjoint extensions [3, 22, 23]. In general, if we ignore the singularity, the resulting Hamiltonian is self-adjoint and positive definite [24], its spectrum is $\mathbb{R}^+$ and there are no bound states. The situation changes if we consider the delta function because the singularity is physically equivalent to an extraction of a single point from the plane $\mathbb{R}^2$, which leads to the loss of the self-adjointness of the Hamiltonian. This has important consequences in the spectrum of the system [25]. However, the self-adjointness is necessary to have a unitary time evolution. So, we must guarantee that the Hamiltonian is self-adjoint, which here is done employing the self-adjoint extension of symmetric operators. With this approach, a new family of self-adjoint operators labeled by a real parameter is obtained.

The situation discussed above occurs, for instance, in the AB scattering of a spin-1/2 particle, where it is well-known that for all real values of the self-adjoint extension parameter, there is an additional scattering amplitude [6], which results from the interaction between the spin and the magnetic flux tube [26]. Moreover, there is one bound state solution with negative energy when this parameter is <0. This situation can be considered quite strange, however, it can be mathematically proved the existence of this negative eigenvalue [3, 5, 27–36]. It is interesting to comment that in reference [29], an equivalence between the renormalization and the self-adjoint extension is discussed.

In this paper, we review some elements of the self-adjoint extension theory which are necessary to address singular Hamiltonians in relativistic and non-relativistic quantum theory. As an application, we consider the model of a spin-1/2 particle with an anomalous magnetic moment in an AB potential in the cosmic string spacetime. As already mentioned above, in this model, a δ function potential arises in the equation of motion [4]. We derive the Dirac equation for this model and solve it for the scattering and bound states on the non-relativistic limit using the self-adjoint extension method. The main goal is to study the physical implications of both the cosmic string background and singularity on the properties of the system. Our application example is motivated by the importance of studying cosmic strings [37], which has been the usual framework for investigating the effects of localized curvature in physical systems. There is a significant number of articles in the literature that study the influence of topology on physical systems using the cosmic string as a background.

Recently, a detailed study to study geometric phase for an open system of a two-level atom interacting with a massless scalar field in the background spacetime of the cosmic string spacetime with torsion was proposed in reference [38]. The authors showed that the geometric phase depends not only on the inherent properties of the atom, but also on the topological properties of background spacetime. For this model, it was found that the correction to the geometric phase of the present system derives from a composite effect, which contains the cosmic string and screw dislocation associated with the curvature and torsion, respectively. The authors also showed that the phase depends on the initial state of this atom and, in particular, there is no geometric phase acquired for the atom if the initial state is prepared in the excited state. Another physical model of current interest that has several studies in cosmic string spacetime is the Dirac oscillator [39]. It is known that the Dirac oscillator is a kind of tensor coupling with a linear potential which leads to the simple harmonic oscillator with a strong spin-orbit coupling problem in the non-relativistic limit. The Dirac oscillator is an exactly soluble model and can be an excellent example in the context of many-particle models in relativistic and non-relativistic quantum mechanics [40]. In reference [41], it was studied the relativistic quantum dynamics of a Dirac oscillator subject to a linear interaction for spin-1/2 particles in a cosmic string spacetime. The authors showed in this model that the geometric and topological properties of these spacetimes lead to shifts in the energy spectrum and the wave-function. In reference [42], the self-adjoint extension method was used to study the effects of spin on the dynamics of a two-dimensional Dirac oscillator in the magnetic cosmic string background. For other important studies in the cosmic string spacetime, the reader may refer to the references [43–46] and in the context of non-relativistic quantum dynamics of a quantum particle constrained to move on a curved surface using da Costa's approach [47] to the references [48–50].

The rest of this work is organized as follows. In section 2 the theory of the self-adjoint extensions is presented and two

different methods, both based on the self-adjoint extension, are discussed. In section 3 the Dirac equation that describes the motion of a spin-1/2 charged particle with an anomalous magnetic moment in the curved space is developed. The methods presented in the previous section are then applied to this system and the scattering and bound states scenarios are discussed. The scattering matrix and the expression for the bound state energy is presented. Finally, in the section 4 we present our conclusions.

2. THE SELF-ADJOINT EXTENSION APPROACH

In this section, we review some important concepts and results from the von-Neumann-Krein theory of self-adjoint extensions. Let A and B two operators. If the domain of A contains the domain of B, i.e., $\mathcal{D}(A) \supseteq \mathcal{D}(B)$, and in the domain of B the operators are equals, then we say that A is an extension of B. The domain of an operator A is called dense if for each vector ψ in this domain, there is a sequence ψ_n in such a way that $\psi_n \to \psi$. If an operator A has a dense domain, the domain of its adjoint $A^\dagger$, is the set of all vectors ψ for which there is a vector $A^\dagger\psi$ that satisfies

$$(\phi, A^\dagger\psi) = (A\phi, \psi), \tag{1}$$

for all vectors $\phi \in \mathcal{D}(A)$. Equation (1) defines $A^\dagger\psi$. On the other hand, an operator with dense domain A is symmetric if

$$(\phi, A\psi) = (A\phi, \psi), \tag{2}$$

for every ϕ and ψ in its domain. In this case $A^\dagger\psi$ is defined as $A^\dagger\psi = A\psi$ for all $\psi \in \mathcal{D}(A)$, and $A^\dagger$ is said to be an extension of A. If $A^\dagger = A$, then A is called self-adjoint or Hermitian. It is interesting to comment that in physics it is common to assume that Hermitian is the same as self-adjointness. However, they are different notions in mathematics literature and only the word Hermitian could be used for symmetric.

An important point here is that a symmetric operator can fail to be a self-adjoint operator. For A to be a self-adjoint operator it has to be symmetric, $A = A^\dagger$, and the domains of the operator and its adjoint have to be equal as well, $\mathcal{D}(A) = \mathcal{D}(A^\dagger)$. So, in the same way as a function needs a rule, a domain and a codomain to be defined, an operator needs not only its action but also its domain (Hilbert space) to be completely defined. Several traditional textbooks on quantum mechanics [51–54] do not mention the problems that could arise by the incorrect or incomplete definition of the operators. An exception being the textbook of the author Ballentine [55]. The mathematical framework of quantum mechanics is that of linear operators in Hilbert spaces and the problems and paradoxes that could arise come from the use of simplified rules described in many textbooks. As an example of this is the use of the theory if bounded operators to deal with unbounded operators [56].

2.1. The Weyl-Von Neumann's Theorem

Following the concept of self-adjoint extension, the question we want to answer is how many extensions, if any, are admitted by an operator. The answer to this question lies in the concept of deficiency index of an operator. Let A be a symmetric operator with domain $\mathcal{D}(A)$ and the corresponding adjoint operator $A^\dagger$ with domain $\mathcal{D}(A^\dagger)$. The deficiency subspaces $\mathcal{N}_\pm$ are defined by [56]

$$\mathcal{N}_\pm = \left\{\psi_\pm \in \mathcal{D}(A^\dagger), \quad A^\dagger\psi_\pm = z_\pm\psi_\pm, \quad Im(z_\pm) \gtrless 0\right\}, \tag{3}$$

with dimensions $\dim\{\mathcal{N}_\pm\} = n_\pm$. The pair of non-negative integers (n_+, n_-) are called deficiency indices of A. The exact value of $z_\pm$ is not important as long as z_+ (z_-) belongs to the upper (lower) half complex plane. For simplicity, it is chosen as $z_\pm = \pm iz_0$, with z_0 an arbitrary positive real number, used for dimensional reasons. In this manner, to access the deficiency indices, all we have to do is to solve the eigenvalue equation

$$A^\dagger\psi_\pm = \pm iz_0\psi_\pm, \tag{4}$$

and then count the number of linearly independent solutions that belong to the domain of the adjoint operator in the Hilbert space in question, i.e., those that are square integrable.

Theorem 1. *(Weyl and Von Neumann [56]) Consider an operator A with deficiency index* (n_+, n_-)*:*

1. *If* $n_+ = n_-$*, A is essentially self-adjoint;*
2. *If* $n_+ = n_- = n \geq 1$*, A posses an infinity number of self-adjoint extensions parameterized by a unitary matrix* $U : \mathcal{N}_+ \to \mathcal{N}_-$ *of dimension n with* n^2 *real parameters;*
3. *If* $n_+ \neq n_-$*, A does not admit a self-adjoint extension.*

Therefore, the domain of $A^\dagger$ is

$$\mathcal{D}(A^\dagger) = \mathcal{D}(A) \oplus \mathcal{N}_+ \oplus \mathcal{N}_-. \tag{5}$$

So, it is important to note that even for Hermitian operators, $A = A^\dagger$, its domains might be different. In this manner, the self-adjoint extension essentially consists of extending the domain of A using the deficiency subspaces $\mathcal{N}_\pm$ to match the domain of $A^\dagger$.

Now that we have discussed some general concepts about the self-adjoint extension approach, we restrict our discussion to the specific case of singular Hamiltonian operators H in (2 + 1) dimensions. In these cases, the singularity is characterized by the presence of a two-dimensional δ function localized at the $r = 0$. It is well-known in the literature that these Hamiltonians are not self-adjoint and admit a one-parameter family of self-adjoint extension [22]. Thus, our main goal is to solve the time-independent Schrödinger equation

$$H\psi = E\psi, \tag{6}$$

with H the Hamiltonian, ψ the wave function and E the energy. To do so, we shall discuss two methods to characterize the family of self-adjoint extensions of H. In both methods, the delta function singularity is replaced by a boundary condition at the origin. In the first one, proposed by Bulla and Gesztesy (BG) in [57], the boundary condition is a mathematical limit allowing divergent solutions for the Hamiltonian H at isolated points, provided they remain square-integrable. In the second one,

proposed by Kay and Studer (KS) in [58], the boundary condition is a match of the logarithmic derivatives of the zero-energy solutions for the regularized Hamiltonian and the solutions for the Hamiltonian H without the delta function plus a self-adjoint extension. As we shall show, the comparison between the results of the two methods allows us to express the self-adjoint extension parameter (a mathematical parameter that characterizes the self-adjoint extension) in terms of the physics of the problem.

2.2. The BG Method

Let us consider the radial singular Schrödinger operator in $L^2((0,\infty))$ given by

$$h = -\frac{d^2}{dr^2} + \frac{\ell(\ell-1)}{r^2} + \frac{\gamma}{r} + \frac{\beta}{r^a} + W, \tag{7}$$

with $W \in L^\infty((0,\infty))$ real valued and $1/2 \leq \ell < 3/2$, $\beta, \gamma \in \mathbb{R}$, $0 < a < 2$. Bulla and Gesztesy showed that this operator, in the interval $1/2 \leq \ell < 3/2$, is not self-adjoint having deficiency indices $(1,1)$. Thus admitting a one-parameter family of self-adjoint extensions. The following theorem characterizes all the self-adjoint extension of h.

Theorem 2. *(Bulla and Gesztesy [3, 57]) All the self-adjoint extension h_ν of h can be characterized by*

$$h_\nu = -\frac{d^2}{dr^2} + \frac{\ell(\ell-1)}{r^2} + \frac{\gamma}{r} + \frac{\beta}{r^a} + W, \tag{8}$$

with domain

$$\mathcal{D}(h_\nu) = \left\{ g \in L^2((0,\infty)) \,|\, g, g' \in AC_{\text{loc}}((0,\infty)); \right. \tag{9}$$

$$\left. -g'' + \frac{\ell(\ell-1)}{r^2} g + \frac{\gamma}{r} g + \frac{\beta}{r^a} g \in L^2((0,\infty)) \right\} \tag{10}$$

with $AC_{\text{loc}}((a,b))$ denoting the set of locally absolutely continuous functions on $((a,b))$ and the function g satisfies the boundary condition

$$\nu g_{0,\ell} = g_{1,\ell}, \tag{11}$$

and

$$-\infty < \nu \leq \infty, \quad \frac{1}{2} \leq \ell < \frac{3}{2}, \quad \beta, \gamma \in \mathbb{R}, \quad 0 < a < 2. \tag{12}$$

The boundary values in (11) are defined by

$$g_{0,\ell} = \lim_{r \to 0^+} \frac{g(r)}{G_\ell^{(0)}(r)}, \tag{13}$$

and

$$g_{1,\ell} = \lim_{r \to 0^+} \frac{g(r) - g_{0,\ell} G_\ell^B(r)}{F_\ell^{(0)}(r)}. \tag{14}$$

The boundary condition $g_{0,\ell} = 0$ (i.e., $\nu = \infty$) represents the Friedrichs extension of h.

The functions $F_\ell^{(0)}(r)$ and $G_\ell^{(0)}(r)$ are given by

$$F_\ell^{(0)}(r) = r^\ell, \tag{15}$$

and

$$G_\ell^{(0)}(r) = \begin{cases} -r^{1/2}\ln(r), & \ell = \frac{1}{2}, \\ \dfrac{r^{1-\ell}}{(2\ell-1)}, & \frac{1}{2} < \ell < \frac{3}{2}. \end{cases} \tag{16}$$

$G_\ell^B(r)$ denotes the asymptotic expansion of $G_\ell(r)$ for $r \to 0^+$ up to r^t, with $t \leq 2\ell - 1$.

2.3. The KS Method

The authors Kay and Studer studied, in the context of self-adjoint extensions, the boundary conditions for singular Hamiltonians in conical spaces and fields around cosmic strings [58]. Among the studied problems, are the AB like problems in two dimensions.

The KS method starts by considering a regularization procedure for the point interaction at the origin. Thus, for the regularized Hamiltonian, where the point interaction is shifted from the origin by a finite very small radius r_0, the method is applied in the following manner [59]:

1. We temporally forget the point interaction at the origin substituting the singular Hamiltonian by the corresponding non-singular one;
2. We solve the Equation (4) for the deficiency spaces of the non-singular Hamiltonian;
3. The solutions obtained in the previous step are used to complete the space of solutions for the non-singular Hamiltonian;
4. In the last step, a boundary condition matching the logarithmic derivatives of the zero-energy solutions for the regularized Hamiltonian of step 1 and the general solutions obtained in step 3 is employed:

$$\lim_{r_0 \to 0^+} r_0 \frac{\dot{g}_0}{g_0}\bigg|_{r=r_0} = \lim_{r_0 \to 0^+} r_0 \frac{\dot{g}_\rho}{g_\rho}\bigg|_{r=r_0}. \tag{17}$$

In the above equation, g_ρ are the solutions obtained in step 3 and g_0 are the zero-energy solutions ($\dot{g} = dg/dr$).

Now that we have discussed the self-adjoint extension approach and the BG and KS methods, in what follows we exemplify the application of both methods to the problem of a spin-1/2 charged particle with an anomalous magnetic moment under the influence of an AB field in conical space.

3. THE DIRAC EQUATION FOR THE AB SYSTEM IN THE CONICAL SPACE

In this section, we shall obtain the Dirac equation to describe the motion of a spin-1/2 charged particle with mass M and anomalous magnetic moment μ_B interacting with an AB field in the cosmic string spacetime. The line element that describes this universe written in cylindrical coordinates is given by

$$ds^2 = dt^2 - dr^2 - \alpha^2 r^2 d\varphi^2 - dz^2, \tag{18}$$

with $-\infty < (t, z) < \infty$, $r \geq 0$ and $0 \leq \varphi \leq 2\pi$. The parameter α in the metric (18) is related to the linear mass density $\bar{m}$ of the cosmic string through the formula $\alpha = 1 - 4\bar{m}$ and it stands for two situations:

- It describes the surface of a cone if $0 < \alpha < 1$. This is equivalent to removing a wedge angle of $2\pi(1-\alpha)$ and the defect presents a positive curvature.
- It describes the surface of an anticone or the figure of a saddle-like surface when $\alpha > 1$. This situation corresponds to the addition of an excess angle of $2\pi(\alpha - 1)$ and, in this case, the defect represents a negative curvature.

In this work, we shall discuss the case of a conical surface, so that $0 < \alpha \leq 1$, with the equality corresponding to the flat space.

The metric in (18) can also be read as the Minkowski spacetime with a conic singularity at $r = 0$ [60]. Because of this characteristic, the only non-zero components of the curvature tensor is found to be

$$R^{r,\varphi}_{r,\varphi} = \frac{1-\alpha}{4\alpha}\delta_2(\mathbf{r}), \tag{19}$$

where $\delta_2(\mathbf{r})$ is the two-dimensional delta function in flat space. The conical singularity in the tensor (19) reveals that the curvature is concentrated on the cosmic string axis and in all other regions it is null.

Since the spacetime is not flat, we must take into account the spin connection in the Dirac equation. To implement this, we need to construct a frame which allows us to obtain the Dirac gamma matrices γ^μ in the Minkowskian spacetime (defined in terms of the local coordinates) in terms of global coordinates. This is done by using the tetrad base $e^{(a)}_{\mu}(x)$, which allows to contract the matrices γ^μ with the inverse tetrad $e^{\mu}_{(a)}(x)$ through the relation

$$\gamma^\mu(x) = e^{\mu}_{(a)}(x)\,\gamma^{(a)}, \tag{20}$$

satisfying the generalized Clifford algebra

$$\left\{\gamma^\mu(x), \gamma^\nu(x)\right\} = 2g^{\mu\nu}(x), \tag{21}$$

with

$$g_{\mu\nu}(x) = e^{(a)}_{\mu}(x)\; e^{(b)}_{\nu}(x)\; \eta_{(a)(b)}, \tag{22}$$

being the metric tensor of the spacetime in the presence of the background topological defect, where $\eta_{(a)(b)}$ is the metric tensor of the flat space, and $(\mu, \nu) = (0, 1, 2, 3)$ represent tensor indices while $(a, b) = (0, 1, 2, 3)$ are tetrad indices. The tetrad and its inverse satisfy the following properties:

$$e^{(a)}_{\mu}(x)\, e^{\mu}_{(b)}(x) = \delta^{(a)}_{(b)} \qquad e^{\mu}_{(a)}(x)\; e^{(a)}_{\nu}(x) = \delta^{\mu}_{\nu}. \tag{23}$$

The matrices $\gamma^{(a)} = \left(\gamma^{(0)}, \gamma^{(i)}\right)$ in Equation (20) are the standard Dirac matrices in Minkowski spacetime, those representation is

$$\gamma^{(0)} = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \gamma^{(i)} = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix}, \quad (i = 1, 2, 3), \tag{24}$$

where $\sigma^i = \left(\sigma^1, \sigma^2, \sigma^3\right)$ are the standard Pauli matrices and I is the 2×2 identity matrix.

To write the generalized Dirac equation in the cosmic string background, we have to take into account the minimal and non-minimal couplings of the spinor to the electromagnetic field embedded in a classical gravitational field. The Dirac equation then reads

$$\Big[i\gamma^\mu(x)\left(\partial_\mu + \Gamma_\mu(x)\right) - e\gamma^\mu(x)\,A_\mu(x) - \frac{a_e\mu_B}{2}\sigma^{\mu\nu}(x)\,F_{\mu\nu}(x) - M\Big]\Psi(x) = 0, \tag{25}$$

where e is the electric charge,

$$a_e = \frac{g_e - 2}{2} = 0,00115965218091, \tag{26}$$

is the anomalous magnetic moment defined, with g_e being the electron's g-factor [61],

$$A_\mu(x) = (A_0, -\mathbf{A}), \tag{27}$$

is the 4-potential of the external electromagnetic field, with $\mathbf{A}$ being the vector potential and A_0 the scalar potential,

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu, \tag{28}$$

is the electromagnetic field tensor whose components are given by

$$\left(F_{0i}, F_{ij}\right) = \left(E^i, \varepsilon_{ijk}B^k\right), \tag{29}$$

and the operator

$$\begin{aligned}\sigma^{\mu\nu}(x) &= \frac{i}{2}[e^{\mu}_{(a)}(x)\,\gamma^{(a)}, e^{\nu}_{(b)}(x)\,\gamma^{(b)}] \\ &= \frac{i}{2}\left[e^{\mu}_{(a)}\gamma^{(a)}e^{\nu}_{(b)}(x)\,\gamma^{(b)} - e^{\nu}_{(b)}(x)\,\gamma^{(b)}e^{\mu}_{(a)}(x)\,\gamma^{(a)}\right],\end{aligned} \tag{30}$$

those components are given by

$$\sigma^{0i} = i\alpha^j = i\begin{pmatrix} 0 & \sigma^i \\ \sigma^i & 0 \end{pmatrix}, \tag{31}$$

$$\sigma^{ij} = -\epsilon_{ijk}\Sigma^k = -\begin{pmatrix} \epsilon_{ijk}\sigma^k & 0 \\ 0 & \epsilon_{ijk}\sigma^k \end{pmatrix}, \tag{32}$$

where

$$\Sigma^k = \begin{pmatrix} \sigma^k & 0 \\ 0 & \sigma^k \end{pmatrix} \tag{33}$$

is the spin operator. The spinor affine connection in Equation (25) is related with the tetrad fields as [62]

$$\Gamma_\mu(x) = \frac{1}{8}\omega_{\mu(a)(b)}(x)\left[\gamma^{(a)}, \gamma^{(b)}\right], \tag{34}$$

where $\omega_{\mu(a)(b)}$ is the spin connection, which can be calculated from the relation

$$\omega_{\mu(a)(b)}(x) = \eta_{(a)(c)} e^{(c)}_{\nu}(x)\, e^{\tau}_{(b)}(x)\, \Gamma^{\nu}_{\tau\mu} - \eta_{(a)(c)} e^{(c)}_{\nu}(x)\, \partial_{\mu} e^{\nu}_{(b)}(x), \tag{35}$$

and $\Gamma^{\nu}_{\tau\mu}$ are the Christoffel symbols.

Now, we need of the tetrad fields to write the Dirac equation in curved space. For the cosmic string spacetime they are chosen to be [63]

$$e^{(a)}_{\mu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\varphi & -\alpha r \sin\varphi & 0 \\ 0 & \sin\varphi & \alpha r \cos\varphi & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$
$$e^{\mu}_{(a)} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\varphi & \sin\varphi & 0 \\ 0 & -\sin\varphi/\alpha r & \cos\varphi/\alpha r & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{36}$$

Using (36), the matrices $\gamma^{\mu}(x)$ in Equation (20) are written more explicitly as

$$\gamma^0 = \beta \equiv \gamma^t, \tag{37}$$
$$\gamma^z \equiv \gamma^z, \tag{38}$$
$$\gamma^1 \equiv \gamma^r = \gamma^{(2)}\cos\varphi + \gamma^{(2)}\sin\varphi, \tag{39}$$
$$\gamma^2 \equiv \frac{\gamma^{\varphi}}{\alpha r} = \frac{1}{\alpha r}\left(-\gamma^{(1)}\sin\varphi + \gamma^{(2)}\cos\varphi\right), \tag{40}$$
$$\gamma^3 \equiv \gamma^z. \tag{41}$$

The matrices (37)–(40) satisfy condition $\nabla_{\mu}\gamma^{\mu} = 0$, which means that they are covariantly constant. The Pauli matrices σ^i in Equation (31) have the following representation:

$$\sigma^r = \begin{pmatrix} 0 & e^{-i\varphi} \\ e^{i\varphi} & 0 \end{pmatrix}, \tag{42}$$
$$\sigma^{\varphi} = \frac{1}{\alpha r}\begin{pmatrix} 0 & -ie^{-i\varphi} \\ ie^{i\varphi} & 0 \end{pmatrix}. \tag{43}$$

Using the basis tetrad (36), the affine connection (34) is found to be [64]

$$\mathbf{\Gamma} = \left(0, 0, \Gamma_{\varphi}, 0\right), \tag{44}$$

where

$$\Gamma_{\varphi} = \frac{1}{2}(1-\alpha)\,\gamma_{(1)}\gamma_{(2)} = -i\frac{(1-\alpha)}{2}\sigma^z, \tag{45}$$

arises as the only non-zero component.

For simplicity, let us assume that the particle interacts with the AB potential, which is generated by a solenoid along the z direction. Since the motion is translationally invariant along this direction, we require that $p_z = z = 0$ and, in Equation (29), we take $E^i = 0$ for $i = 1, 2, 3$. Thus, the particle has a purely planar motion. Equation (25) takes the form

$$\left[-i\partial_0 + \alpha\cdot\left[\frac{1}{i}(\nabla_{\alpha} + \Gamma) - e\mathbf{A}\right] - a_e\mu_B\gamma^0\Sigma\cdot\mathbf{B} + \gamma^0 M\right]\Psi(x) = 0. \tag{46}$$

It is well-known that, in the non-relativistic limit, the large energy M is the driving term in Equation (46). So, writing

$$\Psi = e^{-iEt}\begin{pmatrix} \chi \\ \Phi \end{pmatrix}, \tag{47}$$

we obtain the coupled equations system

$$\sigma\cdot\left[\frac{1}{i}(\nabla_{\alpha} + \Gamma) - e\mathbf{A}\right]\Phi = (i\partial_0 + a_e\mu_B\sigma\cdot\mathbf{B})\,\chi, \tag{48}$$
$$\sigma\cdot\left[\frac{1}{i}(\nabla_{\alpha} + \Gamma) - e\mathbf{A}\right]\chi = (i\partial_0 - a_e\mu_B\sigma\cdot\mathbf{B} + 2M)\,\Phi. \tag{49}$$

On the right side of Equation (49), if we assume that $2M \gg (i\partial_0 - a_e\mu_B\sigma\cdot\mathbf{B})$, we solve it as

$$\Phi = \frac{1}{2M}\sigma\cdot\left[\frac{1}{i}(\nabla + \Gamma) - e\mathbf{A}\right]\chi. \tag{50}$$

Substituting (50) into (48), we get

$$\frac{1}{2M}\sigma\cdot\left[\frac{1}{i}(\nabla_{\alpha} + \Gamma) - e\mathbf{A}\right]\sigma\cdot\left[\frac{1}{i}(\nabla + \Gamma) - e\mathbf{A}\right]\chi - a_e\mu_B\sigma\cdot\mathbf{B}\chi = i\partial_0\chi. \tag{51}$$

Using the relation for Pauli's matrices

$$(\sigma\cdot\mathbf{a})(\sigma\cdot\mathbf{b}) = \mathbf{a}\cdot\mathbf{b} + i\sigma\cdot(\mathbf{a}\times\mathbf{b}), \tag{52}$$

where $\mathbf{a}$ and $\mathbf{b}$ are arbitrary vectors, Equation (51) becomes

$$\frac{1}{2M}\left[\frac{1}{i}(\nabla_{\alpha} + \Gamma) - e\mathbf{A}\right]^2\chi - \frac{e}{2M}(1 + a_e)\,\sigma\cdot\mathbf{B}\chi = i\partial_0\chi. \tag{53}$$

Now we need to define the field configuration. We consider the magnetic field generated by an infinity long cylindrical solenoid in the metric (18). Thus, in the Coulomb gauge, the vector potential reads

$$e\mathbf{A} = -\frac{e\Phi}{2\pi\alpha r}\hat{\boldsymbol{\varphi}} = -\frac{\phi}{\alpha r}\hat{\boldsymbol{\varphi}}, \qquad A_0 = 0, \tag{54}$$

and

$$e\mathbf{B} = -\frac{e\Phi}{2\pi\alpha}\frac{\delta(r)}{r}\hat{\mathbf{z}} = -\frac{\phi}{\alpha}\frac{\delta(r)}{r}\hat{\mathbf{z}}, \tag{55}$$

with $\phi = \Phi/\Phi_0$ being the magnetic flux and $\Phi_0 = 2\pi/e$ is the quantum of magnetic flux. As we can observe, this magnetic field is singular at the origin. The presence of this singularity (a point interaction) in the Hamiltonian, demands that it must be treated by some kind of regularization or, more appropriately, by

using the self-adjoint extension approach. We can note that χ in Equation (53) is an eigenfunction of σ^z, with eigenvalues $s = \pm 1$. In this way, we can write $\sigma^z \chi = \pm\chi = s\chi$. We can take the solutions in the form

$$\chi(t, r, \varphi) = e^{-iEt} \begin{pmatrix} \chi_+(r, \varphi) \\ \chi_-(r, \varphi) \end{pmatrix} = e^{-iEt} \chi_s(r, \varphi). \tag{56}$$

Substituting (45), (54), (55), and (56) in Equation (53), we obtain

$$\frac{1}{2M}\left[\frac{1}{i}\nabla_\alpha - \frac{(1-\alpha)}{2\alpha r} s\hat{\boldsymbol{\varphi}} + \frac{\phi}{\alpha r}\hat{\boldsymbol{\varphi}}\right]^2 \chi_s + \frac{1}{2M}\frac{g_e s\phi}{2\alpha}\frac{\delta(r)}{r}\chi_s(r, \varphi) = E\chi_s(r, \varphi). \tag{57}$$

Therefore, the eigenvalues equation associated with Equation (25) is ($k^2 = 2ME$)

$$H\chi_s = k^2\chi_s, \tag{58}$$

with

$$H = \left[-i\nabla_\alpha - \frac{(1-\alpha)}{2\alpha r} s\hat{\boldsymbol{\varphi}} + \frac{\phi}{\alpha r}\hat{\boldsymbol{\varphi}}\right]^2 + \frac{g_e s\phi}{2\alpha}\frac{\delta(r)}{r}. \tag{59}$$

By expanding the above equation, we arrive at the Laplace-Beltrami operator in the curved space

$$\nabla_\alpha^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{\alpha^2 r^2}\frac{\partial^2}{\partial \varphi^2}. \tag{60}$$

In the present system, the total angular momentum is the sum of the angular momentum and the spin, $J = -i\partial/\partial\varphi + s/2$. Since J commutes with H, we seek solutions of the form

$$\chi_s = \sum_m \psi_m(r)\, e^{im\varphi}, \tag{61}$$

with $m = 0, \pm 1, \pm 2, \pm 3, \ldots$ being the angular momentum quantum number and $\psi_s(r)$ satisfies the differential equation

$$h\psi_m(r) = k^2\psi_m(r), \tag{62}$$

with

$$h = h_0 + \lambda\frac{\delta(r)}{r}, \tag{63}$$

and

$$h_0 = -\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \frac{j^2}{r^2}. \tag{64}$$

The parameter j represents the effective angular momentum

$$j = \frac{m+\phi}{\alpha} - \frac{(1-\alpha)s}{2\alpha}, \tag{65}$$

and

$$\lambda = \frac{g_e\phi s}{2\alpha}. \tag{66}$$

By observing equation (65), one can verify that the presence of the spin element in the model leads to the appearance of a δ function potential. The quantity $\lambda\delta(r)/r$ in Equation (63) is interpreted as the interaction between the spin of the particle and the AB flux tube. As pointed out by Hagen [6, 7] in flat space ($\alpha = 1$), this interaction affects the scattering phase shift. In this work, by using the self-adjoint extension approach, we shall confirm these results and show that this delta function also leads to bound states. This approach had to be adopted to deal with singular Hamiltonians in previous works as, for example, in the study of spin 1/2 AB system and cosmic strings [5, 65], in the Aharonov-Bohm-Coulomb problem [33, 34, 66, 67], and the study of the equivalence between the self-adjoint extension method and renormalization [29].

3.1. Application of the BG Method

In this section, we employ the KS method to find the S-matrix and from its poles we obtain an expression for the bound states. To apply the BG method, we need first transform the operator h_0 in (64) to compare with the form in Equation (7). This is accomplished by employing a similarity transformation by means of the unitary operator $U : L^2(\mathbb{R}^+, rdr) \to L^2(\mathbb{R}^+, dr)$, given by $(U\xi)(r) = r^{1/2}\xi(r)$. Thus, the operator h_0 becomes

$$\tilde{h}_0 = UH_0U^{-1} = -\frac{d^2}{dr^2} + \left(j^2 - \frac{1}{4}\right)\frac{1}{r^2}, \tag{67}$$

and by comparing with (7) we must have $\gamma = \beta = W = 0$ and

$$\ell(\ell - 1) = j^2 - \frac{1}{4}. \tag{68}$$

It is well-known that the radial operator h_0 is not essentially self-adjoint for $\ell(\ell - 1) < 3/4$, otherwise it is essentially self-adjoint [22]. Therefore, using the above equation in this inequality, we have

$$|j| < 1. \tag{69}$$

Before we going to the application of Theorem 2, it is interesting to get a deeper understanding of the significance of the above equation for it informs us for which values of the angular momentum quantum number m the operator h_0 is not self-adjoint. From Equation (65), we see that these values are dependent on the magnetic quantum flux ϕ, the value of α and the spin parameter s. By employing the decomposition of the magnetic quantum flux as

$$\phi = N + \beta, \tag{70}$$

with N being the largest integer contained in ϕ and

$$0 \leq \beta < 1, \tag{71}$$

the inequality in Equation (69), becomes

$$\pi_-^{\mathrm{AB}}(\alpha, \beta) < m < \pi_+^{\mathrm{AB}}(\alpha, \beta), \tag{72}$$

with

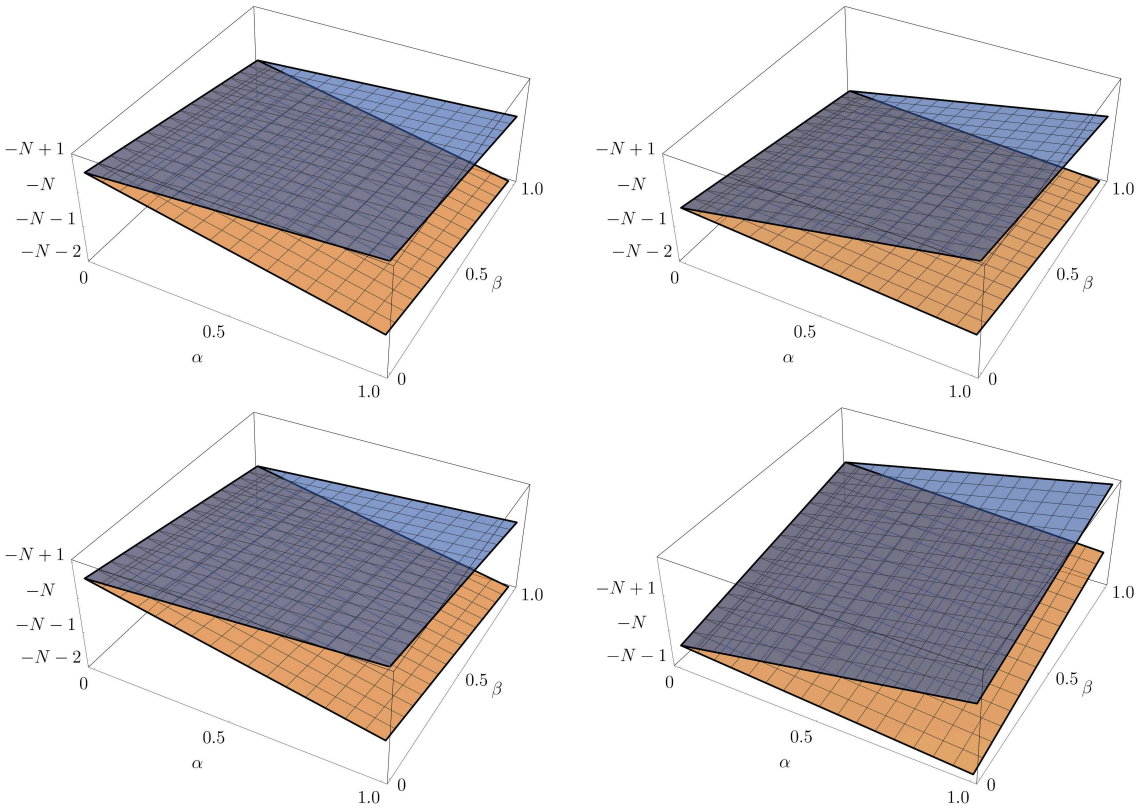

FIGURE 1 | In this figure we show the graphs of the planes $\pi_{\pm}^{AB}(\alpha,\beta)$ for the AB (top panel) and the planes $\pi_{\pm}^{AC}(\alpha,\beta)$ for the AC (bottom panel) effects. The figures on the left are for $s=-1$ and on the right is for $s=+1$. The planes delimit the region where h_0 is not self-adjoint.

$$\pi_{\pm}^{\mathrm{AB}}(\alpha,\beta)=\pm\alpha-(N+\beta)+\frac{(1-\alpha)s}{2}. \tag{73}$$

The planes $\pi_{\pm}^{\mathrm{AB}}(\alpha,\beta)$ delimit the region in which h_0 is not self-adjoint. Given the exact equivalence of the spin 1/2 AB and AC effects [68], Equation (73) should be compared with the corresponding planes obtained for the AC effect in the conical space. In reference [14] it was shown that the planes for the AC effect are given by[1]

$$\pi_{\pm}^{\mathrm{AC}}(\alpha,\beta)=\pm\alpha-s(N+\beta)+\frac{(1-\alpha)s}{2}. \tag{74}$$

Although the equations for the planes are very similar, there is an additional dependence on the spin parameter s in the AC effect. In **Figure 1** we show the planes for AB (top panel) and AC (bottom panel) effects as a function of β and it is possible to see in the AB effect the s parameter changes the values of m in which h_0 is not self-adjoint and the planes are decreasing functions of β whatever the value of s while in the AC effect, besides of changing the values of m, it also controls the inclination of the planes (compare the figures at the bottom panel of **Figure 1**). We can have even more information about the affected m values (in the sense of which values of it h_0 is not self-adjoint) by looking at some specific values of α. Thus, in **Figures 2**, **3** we show cross sections of **Figure 1** for $s=-1$ and $s=+1$, respectively. In **Figures 2**, **3** we can see that for $s=-1$ ($s=+1$) and $\alpha=0.25$ only for $m=-N-1$ ($m=-N$) the operator h_0 is not self-adjoint. On the other hand, for $\alpha=0.50$ for both values of $m=-N$ and $m=-N-1$ the operator h_0 is not self-adjoint. In fact, the minimum value of α in which h_0 is not self-adjoint for both values of m is $\alpha_{\min}=1/3$. Moreover, for $\alpha=1$ (flat space), the operator h_0 is not self-adjoint for both values of angular momentum for all range of β, which is a very well-known result [3, 69–71].

Now that we have discussed in detail the significance of inequality $|j|<1$, we can return to our main discussion. Thus, in the subspace where $|j|<1$, we must apply Theorem 2, in such a way that all the self-adjoint extensions $h_{0,\nu}$ of h_0 are characterized by the boundary condition at the origin

$$\nu\psi_{0,j}=\psi_{1,j}, \tag{75}$$

with $-\infty<\nu\leq\infty$, $-1<j<1$ and the boundary values are

$$\psi_{0,j}=\lim_{r\to0^+}r^{|j|}\psi_m(r),$$
$$\psi_{1,j}=\lim_{r\to0^+}\frac{1}{r^{|j|}}\left[\psi_m(r)-\psi_{0,j}\frac{1}{r^{|j|}}\right].$$

[1]There is a missprint in the signal of the term sN in $\pi_{\pm}(\alpha,\beta)$ in reference [14].

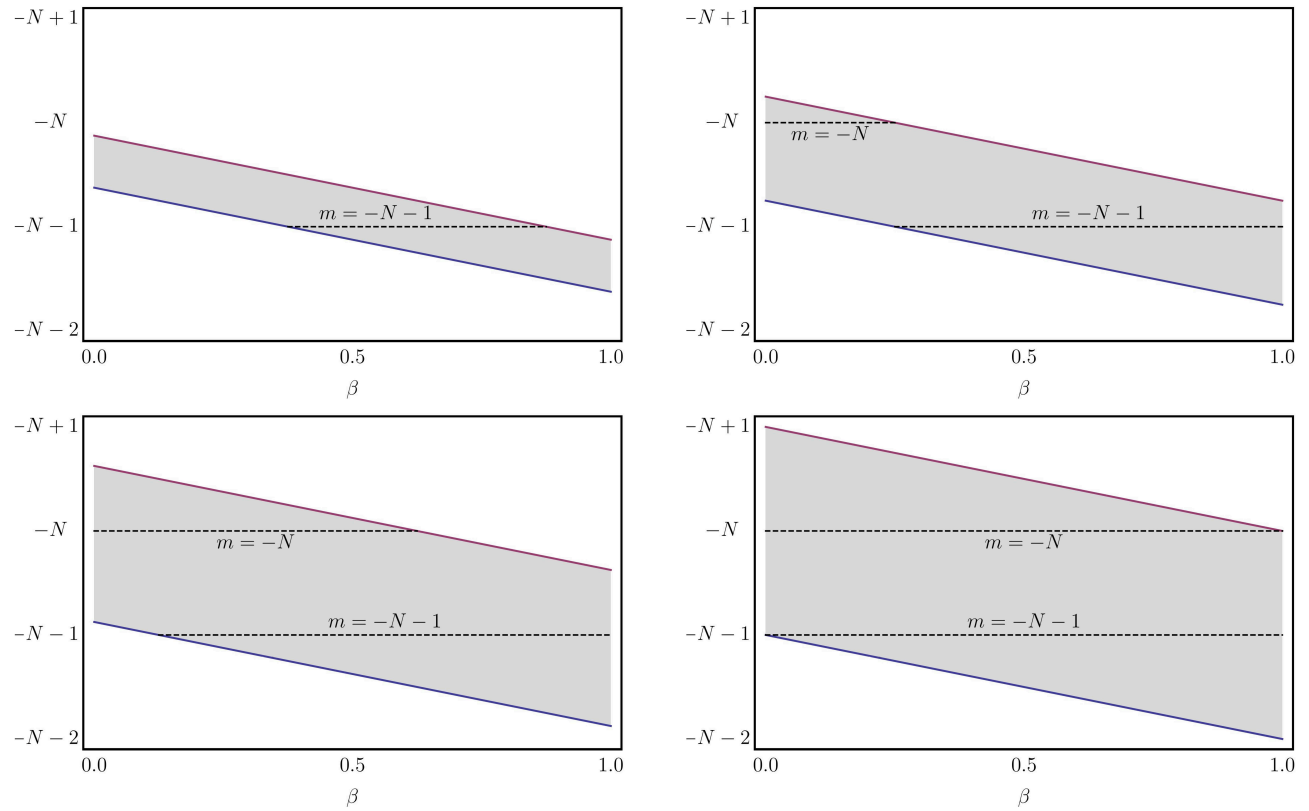

FIGURE 2 | Cross sections of **Figure 1** (top left panel) with $s = -1$ for: α = 0.25 (top left panel), α = 0.50 (top right panel), α = 0.75 (bottom left panel), and α = 1 (bottom right panel). The area of the stripe detached in the figure represents the region in which the operator h_0 is not self-adjoint. The dashed lines refer to the values of angular momentum quantum number.

Physically, it turns out that we can interpret $1/\nu$ as the scattering length of $h_{0,\nu}$ [3]. For $\nu = \infty$ (the Friedrichs extension of h_0), we obtain the free Hamiltonian (the case describing spinless particles) with regular wave functions at the origin ($\psi_m(0) = 0$). This scenario is similar to imposing the Dirichlet boundary condition on the wave function and recovers the original result of Aharanov and Bohm [4]. On the other hand, if $|\nu| < \infty$, $h_{0,\nu}$ characterizes a point interaction at $r = 0$ and the boundary condition permits a $r^{-|j|}$ singularity in the wave functions at this point [72].

Now that we have a suitable boundary condition, we can return to Equation (62) and look for its solutions. Equation (62) is nothing more than the Bessel differential equation for $r \neq 0$. Thus, the general solution for $r \neq 0$ is given by

$$\psi_m(r) = a_m J_{|j|}(kr) + b_m J_{-|j|}(kr), \tag{76}$$

where $J_\nu(z)$ is the Bessel function of fractional order and a_m and b_m are the coefficients corresponding to the contributions of the regular and irregular solutions at $r = 0$, respectively. By means of the boundary condition in Equation (75), we obtain a relation between a_m and b_m,

$$b_m = -\mu_\nu a_m, \tag{77}$$

which is valid in the subspace $|j| < 1$. The term μ_ν is given by

$$\mu_\nu = \frac{k^{2|j|}\Gamma(1-|j|)\sin(|j|\pi)}{4^{|j|}\Gamma(1+|j|)\nu + k^{2|j|}\Gamma(1-|j|)\cos(|j|\pi)}, \tag{78}$$

where $\Gamma(z)$ is the gamma function. In Equation (78) one can verify that μ_ν controls, through ν, the contribution of the irregular solution $J_{-|j|}$ for the wave function. Thus, the solution in this subspace reads

$$\psi_m(r) = a_m \left[J_{|j|}(kr) - \mu_\nu J_{-|j|}(kr)\right]. \tag{79}$$

We can observe that for $\nu = \infty$, we obtain $\mu_\infty = 0$ and, in this case, there is no contribution of the irregular solution at the origin for the wave function. Consequently, in this case, the total wave function becomes

$$\psi = \sum_{m=-\infty}^{\infty} a_m J_{|j|}(kr) e^{im\varphi}. \tag{80}$$

The coefficient a_m in Equation (80) must be chosen in such a way that ψ represents a plane wave that is incident from the right. In this case, we find the following result:

$$a_m = e^{-i|j|\pi/2}. \tag{81}$$

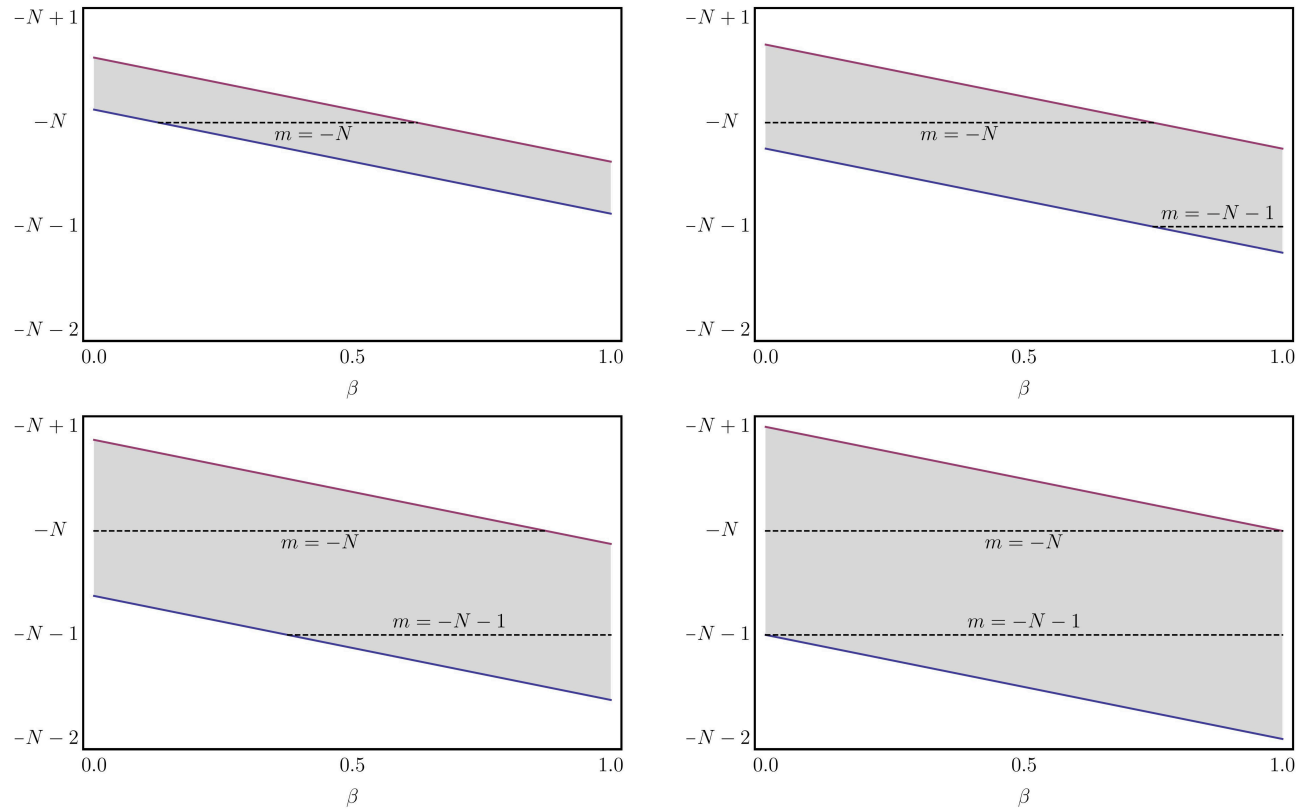

FIGURE 3 | Cross sections of **Figure 1** (top left panel) with $s = +1$ for: $\alpha = 0.25$ (top left panel), $\alpha = 0.50$ (top right panel), $\alpha = 0.75$ (bottom left panel), and $\alpha = 1$ (bottom right panel). The area of the stripe detached in the figure represents the region in which the operator h_0 is not self-adjoint. The dashed lines refer to the values of angular momentum quantum number.

The scattering phase shift can be obtained from the asymptotic behavior of Equation (80). This leads to

$$\delta_m = \frac{\pi}{2}(|m| - |j|). \tag{82}$$

This is the scattering phase shift of the AB effect in the cosmic string spacetime [26, 59]. It is important to mention that, for $\alpha = 1$, it reduces to the phase shift for the usual AB effect in flat space $\delta_m^{AB} = \pi(|m| - |m + \phi|)/2$ [4].

On the other hand, for $|\nu| < \infty$, the contribution of the irregular solution changes the scattering phase shift to

$$\delta_m^{\nu} = \delta_m + \arctan(\mu_\nu). \tag{83}$$

Thus, from standard results for the S-matrix, one obtains

$$S_m^{\nu} = e^{2i\delta_m^{\nu}} = e^{2i\delta_m}\left(\frac{1 + i\mu_\nu}{1 - i\mu_\nu}\right), \tag{84}$$

which is the expression for the S-matrix given in terms of phase shift. It can be seen in (84) that there is an additional scattering for any value of the self-adjoint extension parameter ν. By choosing $\nu = \infty$, we find the S-matrix for the AB effect in the cosmic string spacetime, as it should be.

Having obtained the S-matrix, the bound state energies can be identified as the poles of it in the upper half of the complex k plane. To find them, we need to examine the zeros of the denominator in Equation (84), $1 - i\mu_\nu$, with the replacement $k \to i\kappa_b$ with $\kappa_b = \sqrt{2ME_b}$. Therefore, for $\nu < 0$, the bound state energy is given by

$$E_b = -\frac{2}{M}\left[-\nu\frac{\Gamma(1 + |j|)}{\Gamma(1 - |j|)}\right]^{1/|j|}. \tag{85}$$

Thus, for a fixed negative value of the self-adjoint extension parameter ν, there is a single bound state and the value $2|\nu|^{1/|j|}/M$ fixes the energy scale. The result in Equation (85) coincides with the bound state energy found in references [26, 59] for the AB effect in curved space and is similar that one found in contact interactions of anyons [73]. It is also possible to express the S-matrix in terms of the bound state energy. The result is seen to be

$$S_m^{\nu} = e^{2i\delta_m}\left[\frac{e^{2i\pi|j|} - (\kappa_b/k)^{2|j|}}{1 - (\kappa_b/k)^{2|j|}}\right]. \tag{86}$$

It is important to comment that the above results for the scattering matrix and the bound state energy (for $\nu < 0$) are valid only when $|j| < 1$. Moreover, all the results are dependent on a

free parameter, the self-adjoint extension parameter ν. In what follows we shall show that by employing the KS method, we can find an expression relating the self-adjoint extension parameter with physical parameters of the system.

3.2. Application of the KS Method

In this section, we employ the KS approach to find the bound states for the Hamiltonian in Equation (63). Following the discussion in section 2.3, we temporarily forget the δ-function potential in h and substitute the problem in Equation (62) by the eigenvalue equation for h_0,

$$h_0\psi_\rho = k^2\psi_\rho, \tag{87}$$

plus self-adjoint extensions. Here, ψ_ρ is labeled by the parameter ρ of the self-adjoint extension, which is related to the behavior of the wave function at the origin. To turn h_0 into a self-adjoint operator its domain of definition has to be extended by the deficiency subspace, which is spanned by the solutions of the eigenvalue equation (cf. Equation 4)

$$h_0^\dagger\psi_\pm = \pm ik_0^2\psi_\pm, \tag{88}$$

where $k_0^2 \in \mathbb{R}$ is introduced for dimensional reasons. Since h_0 is Hermitian, $h_0^\dagger = h_0$, the only square integrable functions which are solutions of Equation (88) are the modified Bessel functions of second kind,

$$\psi_\pm = K_{|j|}(\sqrt{\mp i}k_0 r), \tag{89}$$

with $Im\sqrt{\pm i} > 0$. These functions are square integrable only in the range $j \in (-1, 1)$, for which h_0 is not self-adjoint. The dimension of such deficiency subspace is thus $(n_+, n_-) = (1, 1)$, in agreement with the results of the previous sections. In this manner, $\mathcal{D}(h_{\rho,0})$ in $L^2(\mathbb{R}^+, rdr)$ is given by the set of functions [22]

$$\psi_\rho(r) = \psi_m(r) + C\left[K_{|j|}(\sqrt{-i}k_0 r) + e^{i\rho}K_{|j|}(\sqrt{i}k_0 r)\right], \tag{90}$$

where $\psi_m(r)$, with $\psi_m(0) = \dot{\psi}_m(0) = 0$, is the regular wave function and the mathematical parameter $\rho \in [0, 2\pi)$ represents a choice for the boundary condition. For different values of ρ, we have different domains for h_0. and the adequate boundary condition will be determined by the physical system [5, 35, 36, 48]. Thus, in this direction, we use a physically motivated regularization for the magnetic field. So, we replace the original potential vector of the AB flux tube by the following one [6–8, 68]

$$e\mathbf{A} = \begin{cases} -\dfrac{\phi}{\alpha r}\hat{\varphi}, & r > r_0, \\ 0, & r < r_0. \end{cases} \tag{91}$$

where r_0 is a length that defines the defect core radius [35, 58], which is a very small radius smaller than the Compton wave length λ_C of the electron [31]. So one makes the replacement

$$\frac{\delta(r)}{r} \to \frac{\delta(r - r_0)}{r_0}. \tag{92}$$

This regularized form for the delta function allows us to determine an expression for ρ. To do so, we consider the zero-energy solutions ψ_0 and $\psi_{\rho,0}$ for h with the regularization in (92) and h_0, respectively,

$$\left[-\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \frac{j^2}{r^2} + \lambda\frac{\delta(r - r_0)}{r_0}\right]\psi_0 = 0, \tag{93}$$

$$\left[-\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \frac{j^2}{r^2}\right]\psi_{\rho,0} = 0. \tag{94}$$

The value of ρ is determined by the boundary condition

$$\lim_{r_0\to 0^+} r_0\frac{\dot{\psi}_0}{\psi_0}\Big|_{r=r_0} = \lim_{r_0\to 0^+} r_0\frac{\dot{\psi}_{\rho,0}}{\psi_{\rho,0}}\Big|_{r=r_0}. \tag{95}$$

The left-hand side of Equation (95) can be obtained by the direct integration of (93) from 0 to r_0. The result seems to be

$$\lim_{r_0\to 0^+} r_0\frac{\dot{\psi}_0}{\psi_0}\Big|_{r=r_0} = \lambda. \tag{96}$$

The right-hand side of Equation (95) is calculated as follows. First, we seek the solutions of the bound states for the Hamiltonian h_0. These solutions will allow us to obtain the solutions of the bound states for h. As before, for the bound state, we consider k as a pure imaginary quantity, $k \to i\kappa_b$. So, we have

$$\left[\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} - \left(\frac{j^2}{r^2} + \kappa_b^2\right)\right]\psi_\rho(r) = 0, \tag{97}$$

The solution for the above equation is the modified Bessel functions

$$\psi_\rho(r) = K_{|j|}(\kappa_b r). \tag{98}$$

Second, we observe that these solutions belong to $\mathcal{D}(h_{\rho,0})$, such that it is of the form (90) for some ρ selected from the physics of the problem. So, we substitute (98) into (90) and compute $\lim_{r_0\to 0^+} r_0\dot{\psi}_\rho/\psi_\rho|_{r=r_0}$ by using the asymptotic representation for $K_\nu(z)$ in the limit $z \to 0$, which is given by

$$K_\nu(z) \sim \frac{\pi}{2\sin(\pi\nu)}\left[\frac{z^{-\nu}}{2^{-\nu}\Gamma(1-\nu)} - \frac{z^\nu}{2^\nu\Gamma(1+\nu)}\right]. \tag{99}$$

After a straightforward calculation, we have the relation

$$\lim_{r_0\to 0^+} r_0\frac{\dot{\psi}_{\rho,0}}{\psi_{\rho,0}}\Big|_{r=r_0} = \frac{|j|\left[r_0^{2|j|}\Gamma(1-|j|)(\kappa_b/2)^{|j|} + 2^{|j|}\Gamma(1+|j|)\right]}{r_0^{2|j|}\Gamma(1-|j|)(\kappa_b/2)^{|j|} - 2^{|j|}\Gamma(1+|j|)} = \lambda, \tag{100}$$

where we used Equations (95) and (96). Then, solving the above equation for E_b, we find the sought bound state energy

$$E_b = -\frac{2}{Mr_0^2}\left[\left(\frac{\lambda + |j|}{\lambda - |j|}\right)\frac{\Gamma(1+|j|)}{\Gamma(1-|j|)}\right]^{1/|j|}. \tag{101}$$

Now, that we have the bound state energy obtained from BG and KS methods we can compare their results. Thus comparing (85) with (101) we have the following relation

$$\nu = -\frac{1}{r_0^{2|j|}}\left(\frac{\lambda + |j|}{\lambda - |j|}\right). \tag{102}$$

So, we have obtained a relation between the self-adjoint extension parameter and physical parameters of the system.

4. CONCLUSIONS

In this work, we have discussed the self-adjoint extension approach to deal with singular Hamiltonians in (2 + 1) dimensions. Two different methods, both based on the self-adjoint extension approach were discussed in details. The BG and KS methods were applied to solve the problem of a spin-1/2 charged particle with an anomalous magnetic moment in the curved space. The presence of the spin gives rise to a point interaction, requiring the use of the self-adjoint extension approach to solving the problem. In the BG method, the S-matrix was determined and from its poles, one bound state energy expression was obtained. These results were obtained by imposing a suitable boundary condition and depend on the self-adjoint extension parameter, which can be identified as the inverse of the scattering length of the Hamiltonian. Nevertheless, from the mathematical point of view, this parameter is arbitrary. Then, by applying the KS method, an expression for the bound state energy for the same system was obtained, and it is given in terms of physical parameters of the system. Thus comparing the results from both methods a relation between the self-adjoint extension parameter and physical parameters was obtained.

DATA AVAILABILITY STATEMENT

All datasets generated for this study are included in the article/supplementary material.

AUTHOR CONTRIBUTIONS

FA and ES conceived of the presented idea. VS and RC performed the computations. FA and ES verified the analytical methods. All authors discussed the results and contributed to the final manuscript.

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The Propagators for δ and δ' Potentials With Time-Dependent Strengths

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We study the time-dependent Schrödinger equation with finite number of Dirac δ and δ' potentials with time dependent strengths in one dimension. We obtain the formal solution for generic time dependent strengths and then we study the particular cases for single delta potential and limiting cases for finitely many delta potentials. Finally, we investigate the solution of time dependent Schrödinger equation for δ' potential with particular forms of the strengths.

Keywords: propagator, delta potentials, delta prime potentials, Green's function, time dependent Schrödinger equation

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1. INTRODUCTION

Dirac delta potentials in quantum mechanics have been used to model different physical systems almost since the beginning of quantum mechanics. Kronig Penney model [1] is the well-known example of these models. These potentials are the particular cases of much more general class of potentials, namely point interactions. In one dimension, one rigorous way of defining the point interaction at the origin is based on the self-adjoint extension of the free symmetric Hamiltonian defined on $\mathbb{R} \setminus \{0\}$. In this approach, the initially ill-defined formal δ and δ' function potentials appear naturally as two special cases of point interactions constructed from the self-adjoint extension theory. In general one has a 4 -parameter family of self-adjoint extension in one dimension. The monograph [2] includes a great deal of all the details and summarize the history of the literature about the δ interactions. The review article [3] and the book [4] are also good reference sources about the δ potentials from the physical point of view.

The δ' perturbation of free Hamiltonian $H_0 = -\frac{d^2}{dx^2}$ is defined as a limit of short range potentials in the distributional sense [5–7]. Although there are some controversial issues about δ' interactions (see e.g., [8–11]), they are also getting considerable amount of interest. The ambiguities about δ' interactions have been summarized in a very recent article [11], where the integral form of the Schrödinger equation for δ' potential has been studied based on the work of Kurasov [12]. We also adopt the distributional approach developed by Kurasov [12] for the functions having a discontinuity at the point of δ'. It is possible to overcome these ambiguities by considering different choices, as different type of δ' interactions [13]. Therefore, the different results on the spectrum of δ' potential obtained in [2] and in [8] using the Kurasov's approach -as a special case of $-a\delta(x)+b\delta'(x)$ potential- can be interpreted consistently. In other words, the Kurasov's approach corresponds to different self-adjoint extension of the free Hamiltonian H_0. These self-adjoint extensions are given by matching conditions at the origin (or at the point supporting the perturbation) and two of these matching conditions maybe identified as a δ' interaction and receive the names of non-local

and local δ' interaction, respectively [13]. Both approaches are used to see how the spectrum of the V-shaped potential changes when it is perturbed by $-a\delta(x) + b\delta'(x)$ perturbation in [9, 13]. The scattering, and resonant tunneling for δ' potential in one dimension is also a controversial issue because different results are obtained in the literature [8, 10], depending on whether the δ' interaction is the non-local or the local one. The results obtained in [14–16] for the non-local δ' potential, show that it is opaque for all energies of an incoming beam. However, other authors [17–20] claim that there are discrete energy values in the spectrum of δ' potential which lead to resonant tunneling. As an another physical application, δ' interactions are used to model Casimir effect in [21, 22].

The exact expression of the propagator for one dimensional single Dirac delta potentials have been found in different ways [23–25]. The generalization to two center case have been studied in Cacciari and Moretti [26]. The propagator for general four parameter family of point interactions have been given in Albeverio et al. [27]. Propagators for systems involving δ potentials are also studied from various points of view in references [28–34]. The propagator for derivatives of Dirac delta distribution for constant strengths has been recently studied in Lange [11]. The Cauchy problem for the non-local δ' potential with a time dependent strength has also been studied rigorously in detail [35]. Moreover, time dependent one dimensional point interactions have been studied in Campbell [36] and the exact solution to the initial value problem for Schrödinger equation has been given for some particular form of strength $\lambda(t)$ of the Dirac delta potential. Later on, the system has been investigated in Hmidi et al. [37] more rigorously and the regularity assumptions on $\lambda(t)$ is determined for which the initial value problem defines a unitary strongly continuous dynamical system on $L^2(\mathbb{R})$. Such time-dependent point interactions have been studied rigorously in order to model asymptotic complete ionization and suitable conditions on the function $\lambda(t)$ has been determined for ionization problem [38–41]. The higher dimensional generalizations of the problem have been studied in great detail and summarized in the thesis by Correggi [42]. Transmission properties of a monochromatic beam and wave packets by studying the scattering from the time-dependent δ potential are studied in Martinez and Reichl [43] and Kuhn et al. [32]. Utilizing δ potential with a time dependent coefficient in an infinite well, Baek et al. [44] showed that it is possible to split a wave function which may have applications in statistical mechanics and condensed matter physics. However, it may also lead to philosophical problems [44]. The time dependence of the Dirac delta potentials could also be expressed through the motion of its support [45]. As a physical application, a moving Dirac δ potential is used to describe particle displacement using a standard tunneling microscope [46].

The paper is organized as follows: In section 2, we obtain a formal expression of the propagator for a finite number of Dirac δ potentials with time dependent strengths and solve the time dependent Schrödinger equation for this system. In the following subsections, we investigate one δ potential with time dependent strength in more detail and find the propagator for N Dirac δ potential in the limit that centers are infinitely separated. In section 3, we get an expression of the propagator for a finite number of δ' potentials with time dependent strengths and solve the time dependent Schrödinger equation for this potential. Finally, we elaborate on one δ' case.

2. THE PROPAGATOR FOR *N* DIRAC DELTA POTENTIALS WITH TIME DEPENDENT STRENGTHS

We begin with a one dimensional model in which a free Hamiltonian of the type $H_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$ is perturbed with a time dependent potential

$$V(x,t) = \sum_{j=1}^{N} \lambda_j(t)\delta(x - x_j)\ . \tag{1}$$

The initial value problem of the time-dependent Schrödinger equation for this potential is

$$i\frac{\partial}{\partial t}\psi(x,t) = \left[-\frac{d^2}{dx^2} + \sum_{j=1}^{N} \lambda_j(t)\delta(x - x_j)\right]\psi(x,t)\ , \tag{2}$$

with the given sufficiently smooth function $\psi(x,0)$. Here we have used the units such that $\hbar = 2m = 1$ for simplicity. It is well-known that the Laplace transform is a very useful tool to solve initial value problems so we first take the Laplace transformation of Equation (2) with respect to time variable t and get

$$\bar{\psi}_{xx}(x,s) - i\psi(x,0) + is\bar{\psi}(x,s) = \sum_{j=1}^{N} \delta(x - x_j)\mathcal{L}\left\{\lambda_j(t)\psi(x_j,t)\right\}\ , \tag{3}$$

where $\bar{\psi}(x,s) = \mathcal{L}\left\{\psi(x,t)\right\}$ and $\bar{\psi}_{xx}(x,s) = \mathcal{L}\left\{\frac{\partial^2}{\partial x^2}\psi(x,t)\right\}$.

After this, we take the Fourier transformation of both sides of Equation (3) with respect to the coordinate variable x and get:

$$-k^2\hat{\bar{\psi}}(k,s) - i\hat{\psi}(k,0) + is\hat{\bar{\psi}}(k,s) = \sum_{j=1}^{N} e^{-ikx_j}\mathcal{L}\left\{\lambda_j(t)\psi(x_j,t)\right\}\ , \tag{4}$$

where $\hat{\bar{\psi}}(k,s) = \mathcal{F}(\bar{\psi}(x,s))$ denotes the Fourier transform of $\bar{\psi}(x,s)$ with respect to the variable x. This equation is an algebraic equation for the unknown wave function $\hat{\bar{\psi}}(k,s)$ and the solution is easily obtained as

$$\hat{\bar{\psi}}(k,s) = -\frac{1}{k^2 - is}\left[i\hat{\psi}(k,0) + \sum_{j=1}^{N} e^{-ikx_j}\mathcal{L}\left\{\lambda_j(t)\psi(x_j,t)\right\}\right]\ . \tag{5}$$

Now, we immediately find the inverse Fourier transform of the $\hat{\bar{\psi}}(k,s)$:

$$\bar{\psi}(x,s) = -i\int_{-\infty}^{\infty}\frac{dk}{2\pi}\,\frac{e^{ikx}}{k^2 - is}\,\hat{\psi}(k,0)$$

$$-\sum_{j=1}^{N}\mathcal{L}\left\{\lambda_j(t)\psi(x_j,t)\right\}\int_{-\infty}^{\infty}\frac{dk}{2\pi}\frac{e^{ik(x-x_j)}}{k^2-is}\,. \quad (6)$$

Using $\hat{\psi}(k,0) = \int_{-\infty}^{\infty}dx'\ e^{-ikx'}\psi(x',0)$, the Equation (6) becomes

$$\bar{\psi}(x,s) = -i\int_{-\infty}^{\infty}dx'\ \psi(x',0)\int_{-\infty}^{\infty}\frac{dk}{2\pi}\frac{e^{ik(x-x')}}{k^2-is} - \sum_{j=1}^{N}\mathcal{L}\left\{\lambda_j(t)\psi(x_j,t)\right\}\int_{-\infty}^{\infty}\frac{dk}{2\pi}\frac{e^{ik(x-x_j)}}{k^2-is}\,. \quad (7)$$

The integrals in Equation (7) are easily taken using residue theorem

$$\int_{-\infty}^{\infty}\frac{dk}{2\pi}\frac{e^{ikx}}{k^2-is} = i\frac{e^{i\sqrt{is}|x|}}{2\sqrt{is}}\,, \quad (8)$$

so we obtain

$$\bar{\psi}(x,s) = \frac{1}{2\sqrt{is}}\int_{-\infty}^{\infty}dx'\ e^{i\sqrt{is}|x-x'|}\psi(x',0) - \frac{i}{2\sqrt{is}}\sum_{j=1}^{N}e^{i\sqrt{is}|x-x_j|}\mathcal{L}\left\{\lambda_j(t)\psi(x_j,t)\right\}\,. \quad (9)$$

Now we need to take inverse Laplace transform to obtain the solution of the time dependent equation for the potential $\lambda(t)\delta(x)$. Using the Bromwich contour [47], one can easily find the inversion

$$\mathcal{L}^{-1}\left\{\frac{e^{i\sqrt{is}|x|}}{\sqrt{is}}\right\} = \frac{1}{\sqrt{i\pi t}}\ \exp\left(\frac{ix^2}{4t}\right)\,, \quad (10)$$

and using the convolution theorem we get the formal solution as

$$\psi(x,t) = \int_{-\infty}^{\infty}dx'\ \frac{1}{\sqrt{4\pi it}}\ \exp\left[\frac{i(x-x')^2}{4t}\right]\psi(x',0) - i\sum_{j=1}^{N}\int_0^t dt'\ \frac{\lambda_j(t')\psi(x_j,t')}{\sqrt{4\pi i(t-t')}}\exp\left[\frac{i(x-x_j)^2}{4(t-t')}\right]\,. \quad (11)$$

Although this is an explicit formal expression for $\psi(x,t)$, it is not completely expressed in terms of the initial condition $\psi(x,0)$ and includes the unknown factors $\psi(x_j,t)$. These can be found by simply inserting $x = x_j$ in the formal solution and then solving the resulting coupled Volterra type integral equations

$$\psi(x_j,t) = \int_{-\infty}^{\infty}dx'\ \frac{1}{\sqrt{4\pi it}}\ \exp\left[\frac{i(x_j-x')^2}{4t}\right]\psi(x',0) - i\int_0^t dt'\ \frac{\lambda_j(t')\psi(x_j,t')}{\sqrt{4\pi i(t-t')}} - i\sum_{\substack{k=1\\k\neq j}}^{N}\int_0^t dt'\ \frac{\lambda_k(t')\psi(x_k,t')}{\sqrt{4\pi i(t-t')}}\exp\left[\frac{i(x_j-x_k)^2}{4(t-t')}\right]\,, \quad (12)$$

where we split the term $k = j$ in the summation over k. Since this is not an easy problem for a generic function $\lambda(t)$, we will first investigate for particular cases, where λ is constant and λ is inversely proportional to t. All these results we present in the next subsection is previously obtained by Campbell [36] using a slightly different method, where only one integral transformation with the boundary conditions at the position of δ potential was used.

2.1. Single δ Potential With a Time Dependent Strength

As a particular case of (1), we consider a single delta potential with time-dependent strength

$$V(x,t) = \lambda(t)\delta(x)\,, \quad (13)$$

where $N = 1$ and $x_1 = 0$. We can formally obtain the solution of the time dependent Schrödinger equation for this case using Equation (11)

$$\psi(x,t) = \int_{-\infty}^{\infty}dx'\ \frac{1}{\sqrt{4\pi it}}\ \exp\left[\frac{i(x-x')^2}{4t}\right]\psi(x',0) - i\int_0^t dt'\ \frac{\lambda(t')\psi(0,t')}{\sqrt{4\pi i(t-t')}}\exp\left[\frac{ix^2}{4(t-t')}\right]\,. \quad (14)$$

Actually this result can be directly obtained from the Duhamel's formula [48] for time-dependent Schrödinger equation associated with the Hamiltonian $H = H_0 + V$, where H_0 is self-adjoint free Hamiltonian and V is bounded (or relatively H_0 -bounded with relative bound <1):

$$e^{-itH}|\psi_0\rangle = e^{-itH_0}|\psi_0\rangle + (-i)\int_0^t dt'\ e^{-i(t-t')H_0}Ve^{-it'H}|\psi_0\rangle \quad (15)$$

for every $|\psi_0\rangle = |\psi(t=0)\rangle$. This shows that even if we formally take $V = \lambda(t')|0\rangle\langle 0|$ which corresponds to our Dirac delta potential, one immediately sees that the Duhamel's formula is still formally valid for such singular interactions.

Given the initial condition $\psi(x,0)$ and the function $\lambda(t)$, the function $\psi(0,t)$ can be determined by solving the following integral equation:

$$\psi(0,t) = \int_{-\infty}^{\infty}dx'\ \frac{1}{\sqrt{4\pi it}}\ \exp\left[\frac{ix'^2}{4t}\right]\psi(x',0) - i\int_0^t dt'\ \frac{\lambda(t')\psi(0,t')}{\sqrt{4\pi i(t-t')}}. \quad (16)$$

However, this is in general hard to solve and one usually applies some approximation techniques, e.g., Dyson series [48]. Nevertheless, as shown in Campbell [36], there are cases where one can calculate the Green's function explicitly. We will show two such cases here explicitly. Although Green's functions for these cases are derived in Campbell [36], we repeat these results here for the sake of completeness. Instead of directly solving the above integral equation for particular cases, it is convenient to

start with the Laplace transformed wave function Equation (9) for a single δ potential centered at the origin:

$$\bar{\psi}(x,s) = \frac{1}{2\sqrt{is}}\int_{-\infty}^{\infty} dx'\ e^{i\sqrt{is}|x-x'|}\psi(x',0) - \frac{i}{2\sqrt{is}}e^{i\sqrt{is}|x|}\mathcal{L}\left\{\lambda(t)\psi(0,t)\right\}\ . \tag{17}$$

The cases for constant λ and $\lambda \propto \frac{1}{t}$ are reviewed in **Appendices A** and **B** in detail.

2.2. The Propagator for *N* Dirac δ Potentials in a Limiting Case

When λ_j's are constant, the Laplace transformed wave function $\bar{\psi}(x,s)$ given by (9) becomes

$$\bar{\psi}(x,s) = \frac{1}{2\sqrt{is}}\int_{-\infty}^{\infty} dx'\ e^{i\sqrt{is}|x-x'|}\psi(x',0) - \frac{i}{2\sqrt{is}}\sum_{k=1}^{N}\lambda_k\, e^{i\sqrt{is}|x-x_k|}\bar{\psi}(x_k,s)\ . \tag{18}$$

The unknown functions $\bar{\psi}(x_k,s)$ can be found by evaluating the above expression at $x = x_j$:

$$\bar{\psi}(x_k,s) = \sum_{j=1}^{N}\left[\Phi^{-1}(s)\right]_{kj}\ \bar{\rho}(x_j,s)\ , \tag{19}$$

where

$$\Phi_{kj}(s) = \begin{cases} 1+\frac{i\lambda_j}{2\sqrt{is}} & \text{if } j=k \\ \frac{i\lambda_k}{2\sqrt{is}}e^{i\sqrt{is}|x_j-x_k|} & \text{if } j\neq k \end{cases}\ , \tag{20}$$

and

$$\bar{\rho}(x_k,s) = \frac{1}{2\sqrt{is}}\int_{-\infty}^{\infty} dx'\ e^{i\sqrt{is}|x_k-x'|}\psi(x',0)\ . \tag{21}$$

Substituting (19) into (18), we obtain

$$\bar{\psi}(x,s) = \bar{\rho}(x,s) - \frac{i}{2\sqrt{is}}\sum_{j=1}^{N}\sum_{k=1}^{N}\lambda_k\, e^{i\sqrt{is}|x-x_k|}\left[\Phi^{-1}(s)\right]_{kj}\ \bar{\rho}(x_j,s)\ . \tag{22}$$

Although we have obtained the Laplace transformed wave function $\bar{\psi}(x,s)$, it is not explicitly given since one has to invert the matrix Φ and find the inverse Laplace transform of the resulting expression to get the final solution $\psi(x,t)$. In general, it is difficult to find the inverse Laplace transforms so one may apply some approximation schemes [49]. Moreover, one could use some numerical computations, but we will here simply show the limiting case, where the centers are infinitely far away from each other.

When all the centers are infinitely separated from each other, that is, $|x_j - x_k| \to \infty$, we expect that the off-diagonal elements of the matrix Φ given in (20) vanish, so that

$$\left[\Phi^{-1}(s)\right]_{kj} = \left(\frac{1}{1+\frac{i\lambda_k}{2\sqrt{is}}}\right)\delta_{kj}\ . \tag{23}$$

Then, $\bar{\psi}(x,s)$ can be explicitly found as

$$\bar{\psi}(x,s) = \bar{\rho}(x,s) - i\sum_{j=1}^{N} e^{i\sqrt{is}|x-x_j|}\left(\frac{\lambda_j}{2\sqrt{is}+i\lambda_j}\right)\bar{\rho}(x_j,s)\ , \tag{24}$$

from which the propagator $G(x,x',s)$ reads

$$G(x,x',s) = \frac{e^{i\sqrt{is}|x-x'|}}{2\sqrt{is}} - \sum_{j=1}^{N} e^{i\sqrt{is}|x-x_j|}\left(\frac{\lambda_j}{2\sqrt{s}+\sqrt{i}\lambda_j}\right)\frac{e^{i\sqrt{is}|x_j-x'|}}{2\sqrt{s}}\ . \tag{25}$$

Hence,

$$G(x,x',t) = \frac{1}{2\sqrt{i\pi t}}\exp\left[\frac{i(x-x')^2}{4t}\right] - \sum_{j=1}^{N}\frac{\lambda_j}{4}\exp\left[\frac{\lambda_j}{2}(|x-x_j|+|x_j-x'|)+i\frac{\lambda_j^2}{4}t\right] \operatorname{erfc}\left[\frac{(|x-x_j|+|x_j-x'|)}{2\sqrt{it}}+\sqrt{it}\frac{\lambda_j}{2}\right]\ . \tag{26}$$

This is actually the superposition of the individual propagators associated with single delta centers. This is expected since there is no correlation among the centers when they are far away from each other. Another limiting case is the case where all the centers coincide.

3. THE PROPAGATOR FOR *N* DIRAC δ' POTENTIALS WITH TIME DEPENDENT STRENGTHS

In this section we first obtain a formal solution of the time-dependent Schrödinger equation, where the potential term is chosen formally as

$$V(x,t) = \sum_{i=1}^{N}\lambda_i(t)\delta'(x-x_i)\ . \tag{27}$$

The time dependent Schrödinger equation for this potential is

$$i\frac{\partial}{\partial t}\psi(x,t) = \left[-\frac{d^2}{dx^2}+\sum_{j=1}^{N}\lambda_j(t)\delta'(x-x_j)\right]\psi(x,t)\ . \tag{28}$$

As we mentioned in the introduction we adopt the distributional approach given by [12] for the definition of $\delta'(x)$, for functions having discontinuity at the point of δ'

$$\delta'(x)f(x) = \langle f(0)\rangle\delta'(x) - \langle f_x(0)\rangle\delta(x)\,, \tag{29}$$

where we define $\langle f(y)\rangle = \frac{f(y^+)+f(y^-)}{2}$ and $\langle f_x(y)\rangle = \frac{f_x(y^+)+f_x(y^-)}{2}$ and $f(y^\pm)$ denote the limits $\lim_{x\to y^\pm} f(x)$. Note that this definition reduces to the well-known property of $\delta'(x)$ [50]

$$\delta'(x)f(x) = f(0)\delta'(x) - f'(0)\delta(x)\,. \tag{30}$$

for continuous functions. As in the previous section we proceed by taking the Laplace transform of all the terms in the Equation (28) for time variable t and find

$$\begin{aligned}&\bar{\psi}_{xx}(x,s) - i\psi(x,0) + is\bar{\psi}(x,s)\\ &= \sum_{j=1}^{N}\left[-\mathcal{L}\left\{\lambda_j(t)\langle\psi(x_j)\rangle\right\}\delta'(x-x_j)\right.\\ &\left.+\mathcal{L}\left\{\lambda_j(t)\langle\psi_x(x_j)\rangle\right\}\delta(x-x_j)\right]\,.\end{aligned} \tag{31}$$

Now, we take the Fourier transform with respect to the variable x and solve $\hat{\bar{\psi}}(k,s)$ to get:

$$\begin{aligned}\hat{\bar{\psi}}(k,s) = -\tfrac{1}{k^2-is}\big(i\hat{\psi}(k,0) + \textstyle\sum_{j=1}^{N} -ike^{-ikx_j}\mathcal{L}\left\{\lambda_j(t)\langle\psi(x_j)\rangle\right\}\\ +e^{-ikx_j}\mathcal{L}\left\{\lambda_j(t)\langle\psi_(x_j)\rangle\right\}\big)\,.\end{aligned} \tag{32}$$

Before taking the inverse Fourier transform of this equation we write $\hat{\psi}(k,0) = \int_{-\infty}^{\infty} dx' e^{-ikx'}\psi(x',0)$ then take the inverse Fourier transform and get

$$\begin{aligned}\bar{\psi}(x,s) &= \frac{1}{2\sqrt{is}}\int_{-\infty}^{\infty} dx'\; e^{i\sqrt{is}|x-x'|}\;\psi(x',0)\\ &-\frac{1}{2}\sum_{j=1}^{N}\mathrm{sgn}(x-x_j)\; e^{i\sqrt{is}|x-x_j|}\;\mathcal{L}\left\{\lambda_j(t)\langle\psi(x_j,t)\rangle\right\}\\ &-i\frac{1}{2\sqrt{is}}\sum_{j=1}^{N} e^{i\sqrt{is}|x-x_j|}\;\mathcal{L}\left\{\lambda_j(t)\langle\psi_x(x_j,t)\rangle\right\}\;.\end{aligned} \tag{33}$$

where $\mathrm{sgn}(x)$ denotes sign function $\mathrm{sgn}(x) = \begin{cases}1 & x>0\\ -1 & x<0\end{cases}$. We have also used $\int_{-\infty}^{\infty}\frac{dk}{2\pi}\frac{e^{ikx}}{k^2-is} = -\frac{i}{2\sqrt{is}}e^{i\sqrt{is}|x|}$ and $\int_{-\infty}^{\infty}\frac{dk}{2\pi}\frac{ike^{ikx}}{k^2-is} = -\frac{1}{2\sqrt{is}}e^{i\sqrt{is}|x|}\,\mathrm{sgn}(x)$. Now using $\mathcal{L}\left\{\frac{\exp\left[i\frac{x^2}{4t}\right]}{2\sqrt{i\pi}\,t}\right\} = \frac{e^{i\sqrt{is}|x|}}{2\sqrt{is}}$ and $\mathcal{L}\left\{(-1)^{3/4}\frac{\exp\left[i\frac{x^2}{4t}\right]x}{2\sqrt{\pi}t^{3/2}}\right\} = e^{i\sqrt{is}|x|}\,\mathrm{sgn}(x)$ and convolution theorem for Laplace transform we get the formal expression of the wave function

$$\begin{aligned}\psi(x,t) &= \int_{-\infty}^{\infty} dx'\;\frac{1}{\sqrt{4\pi it}}\;e^{i\frac{(x-x')^2}{4t}}\psi(x',0)\\ &-\int_0^t dt'\left\{\sum_{j=1}^{N}\frac{(-1)^{3/4}}{4\sqrt{\pi}}\lambda_j(t')\langle\psi(x_j)\rangle\frac{\exp\left[i\frac{(x-x_j)^2}{4(t-t')}\right]}{(t-t')^{3/2}}\;(x-x_j)\right.\\ &\left.+\frac{i}{2\sqrt{i\pi}}\sum_{j=1}^{N}\lambda_j(t')\langle\psi_x(x_j)\rangle\frac{\exp\left[i\frac{(x-x_j)^2}{4(t-t')}\right]}{\sqrt{(t-t')}}\right\}\,.\end{aligned} \tag{34}$$

Similar to the time dependent δ potential case, this formal equation contains unknown functions $\psi(x_j^\pm)$'s and $\psi_x(x_j^\pm)$'s. One can find equations for $\psi(x_j^\pm)$'s by inserting $x = x_j^\pm$ to the Equation (34). In order to find equations for $\psi_x(x_j)^\pm$'s, the derivative of the Equation (34) with respect to the variable x has to be calculated. By taking this derivative we get

$$\begin{aligned}\psi_x(x,t) &= \frac{1}{4\sqrt{i\pi}\,t^{3/2}}\int_{-\infty}^{\infty} dx'\;i(x-x')\;e^{i\frac{(x-x')^2}{4t}}\psi(x',0)\\ &-\int_0^t dt'\left\{-\frac{1}{8}\sqrt{\frac{i}{\pi}}\sum_{j=1}^{N}\lambda_j(t')\langle\psi(x_j)\rangle i(x-x_j)^2\frac{\exp\left[i\frac{(x-x_j)^2}{4(t-t')}\right]}{(t-t')^{5/2}}\right.\\ &+\frac{(-1)^{3/4}}{4\sqrt{\pi}}\sum_{j=1}^{N}\lambda_j(t')\langle\psi(x_j)\rangle\frac{\exp\left[i\frac{(x-x_j)^2}{4(t-t')}\right]}{(t-t')^{3/2}}\\ &\left.-\frac{1}{4\sqrt{i\pi}}\sum_{j=1}^{N}\lambda_j(t')\langle\psi_x(x_j)\rangle(x-x_j)\frac{\exp\left[i\frac{(x-x_j)^2}{4(t-t')}\right]}{(t-t')^{3/2}}\right\}\,.\end{aligned} \tag{35}$$

Now putting $x = x_j^\pm$ in the Equation (35) one can get also integral equations for $\psi_x(x_j^\pm)$'s. Finally one has to solve the system of integral equations for $\psi(x_j^\pm)$'s and $\psi_x(x_j^\pm)$'s to get the complete solution.

3.1. Single δ' Potential With a Time Dependent Strength

Now we will elaborate more on the single δ' interaction which is described by the potential

$$V(x,t) = \lambda(t)\delta'(x) \tag{36}$$

The formal solution of the time dependent Schrödinger equation for single δ' can be obtained from the above section for $N=1$, $x_1 = 0$ and $\lambda_1 = \lambda$

$$\begin{aligned}\psi(x,t) &= \int_{-\infty}^{\infty} dx'\;\frac{1}{\sqrt{4\pi it}}\;e^{i\frac{(x-x')^2}{4t}}\psi(x',0)\\ &-\int_0^t dt'\left\{\frac{(-1)^{3/4}}{4\sqrt{\pi}}\lambda(t')\langle\psi(0)\rangle\;x\;\frac{\exp\left[i\frac{x^2}{4(t-t')}\right]}{(t-t')^{3/2}}\right.\\ &\left.+\frac{i}{2\sqrt{i\pi}}\lambda(t')\langle\psi_x(0)\rangle\frac{\exp\left[i\frac{x^2}{4(t-t')}\right]}{\sqrt{(t-t')}}\right\}\,.\end{aligned} \tag{37}$$

Similarly the expression for the $\psi_x(x,t)$ is obtained from the Equation (35)

$$\begin{aligned}\psi_x(x,t) &= \frac{1}{4\sqrt{i\pi}t^{3/2}}\int_{-\infty}^{\infty} dx'\; i(x-x')\; e^{i\frac{(x-x')^2}{4t}}\psi(x',0)\\ &-\int_0^t dt'\left\{-\frac{1}{8}\sqrt{\frac{i}{\pi}}\lambda(t')\langle\psi(0)\rangle\; x^2\;\frac{\exp\left[i\frac{x^2}{4(t-t')}\right]}{(t-t')^{5/2}}\right.\\ &+\frac{(-1)^{3/4}}{4\sqrt{\pi}}\lambda(t')\langle\psi(0)\rangle\frac{\exp\left[i\frac{x^2}{4(t-t')}\right]}{(t-t')^{3/2}}\\ &\left.-\frac{1}{4\sqrt{i\pi}}\lambda(t')\langle\psi_x(0)\rangle\; x\;\frac{\exp\left[i\frac{x^2}{4(t-t')}\right]}{(t-t')^{3/2}}\right\}.\end{aligned} \tag{38}$$

For a given $\lambda(t)$ one gets integral equations for $\psi(x,0)$ and $\psi_x(x,0)$ by inserting $x = 0$ in Equations (37) and (38), respectively:

$$\begin{aligned}\psi(0,t) &= \int_{-\infty}^{\infty} dx'\;\frac{1}{\sqrt{4\pi\, it}}\; e^{i\frac{x'^2}{4t}}\psi(x',0)\\ &-\int_0^t dt'\left\{\frac{(-1)^{3/4}}{4\sqrt{\pi}}\lambda(t')\langle\psi(0)\rangle\frac{1}{(t-t')^{3/2}}\right.\\ &\left.+\frac{i}{2\sqrt{i\pi}}\lambda(t')\langle\psi_x(0)\rangle\frac{1}{\sqrt{(t-t')}}\right\}.\end{aligned} \tag{39}$$

$$\begin{aligned}\psi_x(0,t) &= \tfrac{1}{4\sqrt{i\pi}t^{3/2}}\int_{-\infty}^{\infty} dx'\;(-x')e^{i\frac{x'^2}{4t}}\psi(x',0)\\ &-\tfrac{(-1)^{3/4}}{4\sqrt{\pi}}\int_0^t dt'\;\lambda(t')\langle\psi(0)\rangle\tfrac{1}{(t-t')^{3/2}}.\end{aligned} \tag{40}$$

The Equations (39) and (40) constitute an equation system for $\psi(0,t)$ and $\psi_x(0,t)$. Solving this system one can determine $\psi(0,t)$ and $\psi_x(0,t)$ and insert them to Equation (37) to get the wave function for all times. When studying special cases the expression of the Laplace transform of the wave function is necessary. Therefore, utilizing Equation (33) we write the general formula of the Laplace transform of the wave function for a delta prime at $x_1 = 0$ and $\lambda_1(t) = \lambda(t)$:

$$\begin{aligned}\bar{\psi}(x,s) &= \frac{1}{2\sqrt{is}}\int_{-\infty}^{\infty} dx'\; e^{i\sqrt{is}|x-x'|}\;\psi(x',0)\\ &-\frac{1}{2}\,\mathrm{sgn}(x)\; e^{i\sqrt{is}|x|}\;\mathcal{L}\left\{\lambda(t)\langle\psi(0,t)\rangle\right\}\\ &-i\frac{1}{2\sqrt{is}}e^{i\sqrt{is}|x|}\;\mathcal{L}\left\{\lambda(t)\langle\psi_x(0,t)\rangle\right\}\;.\end{aligned} \tag{41}$$

Now will investigate some special cases.

3.1.1. Case 1: λ Is Constant

When the strength of the single δ' interaction is constant, we obtain from Equation (33)

$$\begin{aligned}\bar{\psi}(x,s) &= \frac{1}{2\sqrt{is}}\int_{-\infty}^{\infty} dx'\; e^{i\sqrt{is}|x-x'|}\;\psi(x',0)\\ &-\frac{\lambda}{2}\,\mathrm{sgn}(x)e^{i\sqrt{is}|x|}\;\langle\psi(\bar{0},s)\rangle\\ &-i\frac{\lambda}{2\sqrt{is}}e^{i\sqrt{is}|x|}\;\langle\psi_x(\bar{0},s)\rangle\;,\end{aligned} \tag{42}$$

where $\langle\bar{\psi}(0,s)\rangle = \mathcal{L}\left\{\langle\psi(x,t)\rangle\right\}$ and $\langle\bar{\psi}_x(0,s)\rangle = \mathcal{L}\left\{\langle\psi_x(x,t)\rangle\right\}$. We need also derivative of the Laplace transformed wave function $\bar{\psi}(x,s)$ with respect to x.

$$\begin{aligned}\bar{\psi}_x(x,s) &= \frac{i}{2}\int_{-\infty}^{\infty} dx'\;\mathrm{sgn}(x-x')\; e^{i\sqrt{is}|x-x'|}\;\psi(x',0)\\ &-\frac{i\lambda\sqrt{is}}{2}\,\mathrm{sgn}^2(x)e^{i\sqrt{is}|x|}\;\langle\psi(\bar{0},s)\rangle\\ &-\frac{\lambda}{2}\frac{d\,\mathrm{sgn}(x)}{dx}e^{i\sqrt{is}|x|}\;\langle\psi(\bar{0},s)\rangle+\frac{\lambda\,\mathrm{sgn}(x)e^{i\sqrt{is}|x|}}{2}\langle\psi_x(\bar{0},s)\rangle\;,\end{aligned} \tag{43}$$

where we have used $\frac{d|x|}{dx} = \mathrm{sgn}(x)$. Now we find wave function and its derivative at $0^{\pm}$ by choosing $x = 0^{\pm}$ in Equations (42) and (43):

$$\begin{aligned}\bar{\psi}(0^{\pm},s) &= \frac{1}{2\sqrt{is}}\int_{-\infty}^{\infty} dx'\; e^{i\sqrt{is}|x'|}\;\psi(x',0)\mp\frac{\lambda}{2}\;\langle\psi(\bar{0},s)\rangle\\ &-\frac{i\lambda}{2\sqrt{is}}\;\langle\psi_x(\bar{0},s)\rangle\;,\end{aligned} \tag{44}$$

where we take $\mathrm{sgn}(0^{\pm}) = \pm 1$. In order to find $\bar{\psi}(x,s)$ we need to calculate $\langle\bar{\psi}(0,s)\rangle$ and $\langle\bar{\psi}_x(0,s)\rangle$. From Equation (44) we get

$$\langle\bar{\psi}(0,s)\rangle+\frac{i\lambda}{2\sqrt{is}}\langle\bar{\psi}_x(0,s)\rangle = \frac{1}{2\sqrt{is}}\int_{-\infty}^{\infty} dx'\; e^{i\sqrt{is}|x'|}\;\psi(x',0)\;. \tag{45}$$

In order to find another equation for $\langle\bar{\psi}(0,s)\rangle$ and $\langle\bar{\psi}_x(0,s)\rangle$ we calculate $\bar{\psi}_x(0^{\pm},s)$

$$\begin{aligned}\bar{\psi}_x(0^{\pm},s) &= \frac{i}{2}\int_{-\infty}^{\infty} dx'\;\mathrm{sgn}(-x')\; e^{i\sqrt{is}|x'|}\;\psi(x',0)\\ &-\frac{i\lambda\sqrt{is}}{2}\;\langle\bar{\psi}(0,s)\rangle\mp\frac{\lambda}{2}\langle\bar{\psi}_x(0,s)\rangle\;.\end{aligned} \tag{46}$$

where we take $\frac{d\,\mathrm{sgn}(x)}{dx}|_{x=0^{\pm}} = 0$. Using this equation we get

$$\frac{i\lambda\sqrt{is}}{2}\langle\bar{\psi}(0,s)\rangle+\langle\bar{\psi}_x(0,s)\rangle = \frac{i}{2}\int_{-\infty}^{\infty} dx'\;\mathrm{sgn}(-x')\; e^{i\sqrt{is}|x'|}\;\psi(x',0). \tag{47}$$

Solving Equations (45) and (47) we get

$$\langle\bar{\psi}(0,s)\rangle = \frac{1}{2\sqrt{is}}\left(1+\frac{\lambda^2}{4}\right)^{-1}$$

$$\int_{-\infty}^{\infty} dx' \left(1 - \frac{\lambda}{2}\,\mathrm{sgn}(x')\right) e^{i\sqrt{is}|x'|}\ \psi(x',0)\,, \tag{48}$$

and

$$\langle\bar{\psi}_x(0,s)\rangle = \int_{-\infty}^{\infty} dx' \left[-\frac{i}{2}\,\mathrm{sgn}(x') - \frac{i\lambda}{4}\left(1+\frac{\lambda^2}{4}\right)^{-1} \left(1 - \frac{\lambda}{2}\,\mathrm{sgn}(x')\right)\right] e^{i\sqrt{is}|x'|}\ \psi(x',0)\,, \tag{49}$$

respectively. Substituting the expressions in Equations (48) and (49) into Equation (42) we get

$$\bar{\psi}(x,s) = \int_{-\infty}^{\infty} dx' \left\{\frac{e^{i\sqrt{is}|x-x'|}}{2\sqrt{is}} + \left(1+\frac{\lambda^2}{4}\right)^{-1}\left[-\frac{\lambda}{4}\,\mathrm{sgn}(x') - \frac{\lambda^2}{8} - \frac{\lambda}{4}\,\mathrm{sgn}(x)\ + \frac{\lambda^2}{8}\,\mathrm{sgn}(x)\ \mathrm{sgn}(x')\right]\frac{e^{i\sqrt{is}(|x|+|x'|)}}{\sqrt{is}}\right\}\psi(x',0)\,. \tag{50}$$

The factor that multiplies $\psi(x',0)$ in the integral of the equation above is the Green's function:

$$\bar{G}(x,x',s) = \left\{\frac{e^{i\sqrt{is}|x-x'|}}{2\sqrt{is}} + \left(1+\frac{\lambda^2}{4}\right)^{-1}\left[-\frac{\lambda}{4}\,\mathrm{sgn}(x') - \frac{\lambda^2}{8} - \frac{\lambda}{4}\,\mathrm{sgn}(x)\ + \frac{\lambda^2}{8}\,\mathrm{sgn}(x)\ \mathrm{sgn}(x')\right]\frac{e^{i\sqrt{is}(|x|+|x'|)}}{\sqrt{is}}\right\}. \tag{51}$$

The Green's function in terms of s variable can be converted using Equation (10) to get

$$G(x,x',t) = \frac{1}{\sqrt{4\pi it}}\left\{e^{i\frac{(x-x')^2}{4t}} + \left(1+\frac{\lambda^2}{4}\right)^{-1}\left[-\frac{\lambda}{2}\,\mathrm{sgn}(x') - \frac{\lambda^2}{4} - \frac{\lambda}{2}\,\mathrm{sgn}(x)\ + \frac{\lambda^2}{4}\,\mathrm{sgn}(x)\ \mathrm{sgn}(x')\right]e^{i\frac{(|x|+|x'|)^2}{4t}}\right\}. \tag{52}$$

So, we can write the wave function for all times as:

$$\psi(x,t) = \frac{1}{\sqrt{4\pi it}}\int_{-\infty}^{\infty} dx' \left\{e^{i\frac{(x-x')^2}{4t}} + \left(1+\frac{\lambda^2}{4}\right)^{-1}\left[-\frac{\lambda}{2}\,\mathrm{sgn}(x') - \frac{\lambda^2}{4} - \frac{\lambda}{2}\,\mathrm{sgn}(x)\ + \frac{\lambda^2}{4}\,\mathrm{sgn}(x)\ \mathrm{sgn}(x')\right] e^{i\frac{(|x|+|x'|)^2}{4t}}\right\}\psi(x',0)\,. \tag{53}$$

This result is completely consistent with the one given in Lange [11] except the convention $\lambda = -c$.

3.1.2. Case 2: $\lambda(t) = \alpha/t$

The general expression (41) for the Laplace transform of the wave function in this particular case $\lambda(t) = \frac{\alpha}{t}$, where α is a constant, becomes

$$\bar{\psi}(x,s) = \frac{1}{2\sqrt{is}}\int_{-\infty}^{\infty} dx'\ e^{i\sqrt{is}|x-x'|}\ \psi(x',0) - \frac{1}{2}\,\mathrm{sgn}(x)\ e^{i\sqrt{is}|x|}\ \mathcal{L}\left\{\frac{\alpha}{t}\langle\psi(0,t)\rangle\right\} - i\frac{1}{2\sqrt{is}}e^{i\sqrt{is}|x|}\ \mathcal{L}\left\{\frac{\alpha}{t}\langle\psi_x(0,t)\rangle\right\}\,. \tag{54}$$

Using the identity given in Equation (B.2) in **Appendix B** this equation becomes

$$\bar{\psi}(x,s) = \frac{1}{2\sqrt{is}}\int_{-\infty}^{\infty} dx'\ e^{i\sqrt{is}|x-x'|}\ \psi(x',0) - \frac{1}{2}\,\mathrm{sgn}(x)\ e^{i\sqrt{is}|x|}\ \alpha\int_s^{\infty} ds'\langle\bar{\psi}(0,s')\rangle - i\frac{1}{2\sqrt{is}}e^{i\sqrt{is}|x|}\ \alpha\int_s^{\infty} ds'\langle\bar{\psi}_x(0,s')\rangle\,. \tag{55}$$

In order to calculate this expression we need $\psi(0^{\pm},s)$ and $\psi_x(0^{\pm},s)$. The first of this is easily calculated by choosing $x = 0^{\pm}$ in Equation (55)

$$\bar{\psi}(0^{\pm},s) = \frac{1}{2\sqrt{is}}\int_{-\infty}^{\infty} dx'\ e^{i\sqrt{is}|x'|}\ \psi(x',0) \mp\frac{\alpha}{2}\int_s^{\infty} ds'\langle\bar{\psi}(0,s')\rangle - \frac{i\alpha}{2\sqrt{is}}\int_s^{\infty} ds'\langle\bar{\psi}_x(0,s')\rangle\,. \tag{56}$$

In order to find $\psi_x(0^{\pm},s)$ we take the derivative of the Equation (54) with respect to x variable and get

$$\bar{\psi}_x(x,s) = \frac{i}{2}\int_{-\infty}^{\infty} dx'\ sgn(x-x')e^{i\sqrt{is}|x-x'|}\ \psi(x',0) - \frac{i\sqrt{is}\alpha}{2}\,\mathrm{sgn}^2(x)\ e^{i\sqrt{is}|x|}\int_s^{\infty} ds'\langle\bar{\psi}(0,s')\rangle - 2e^{i\sqrt{is}|x|}\ \alpha\frac{d\,\mathrm{sgn}(x)}{dx}\int_s^{\infty} ds'\langle\bar{\psi}(0,s')\rangle + \frac{\alpha}{2}\,\mathrm{sgn}(x)e^{i\sqrt{is}|x|}\int_s^{\infty} ds'\langle\bar{\psi}_x(0,s')\rangle\,. \tag{57}$$

From this equation we get

$$\bar{\psi}_x(0^{\pm},s) = -\frac{i}{2}\int_{-\infty}^{\infty} dx'\ \mathrm{sgn}(x')e^{i\sqrt{is}|x'|}\ \psi(x',0) - \frac{i\sqrt{is}\,\alpha}{2}\int_s^{\infty} ds'\langle\bar{\psi}(0,s')\rangle \pm\frac{\alpha}{2}\int_s^{\infty} ds'\langle\bar{\psi}_x(0,s')\rangle\,. \tag{58}$$

We denote $u_1(s) = \int_s^{\infty} ds'\langle\bar{\psi}(0,s')\rangle$ and $u_2(s) = \int_s^{\infty} ds'\langle\bar{\psi}_x(0,s')\rangle$. We obtain from Equations (56) and (58)

$$\langle\bar{\psi}(0,s)\rangle = \frac{I_0(s)}{2\sqrt{is}} - \frac{i\alpha}{2\sqrt{is}}u_1(s) \tag{59}$$

and

$$\langle\bar{\psi}_x(0,s)\rangle = -i\frac{I_1(s)}{2} - \frac{i\sqrt{is}\alpha}{2}u_2(s). \tag{60}$$

Here $I_0(s) = \int_{-\infty}^{\infty} dx'\ \ e^{i\sqrt{is}|x'|}\psi(x',0)$ and $I_1(s) = \int_{-\infty}^{\infty} dx'\ \ \mathrm{sgn}\,x'e^{i\sqrt{is}|x'|}\psi(x',0)$. Note that $\langle\bar{\psi}(0,s)\rangle = -\frac{du_1(s)}{ds}$ and $\langle\bar{\psi}_x(0,s)\rangle = -\frac{du_2(s)}{ds}$. Inserting these equalities into Equations (59) and (60) we obtain two coupled differential equations:

$$\frac{du_1(s)}{ds} - \frac{i\alpha}{2\sqrt{is}}u_2(s) = -\frac{I_0(s)}{2\sqrt{is}} \tag{61}$$

and

$$\frac{du_2(s)}{ds} - \frac{i\sqrt{is}\alpha}{2}u_1(s) = i\frac{I_1(s)}{2\sqrt{is}}\,. \tag{62}$$

Although the coefficients of the unknown functions are not constants in these coupled equations, by taking the derivative of the Equations (61) and (62) with respect to the variable s one can uncouple these equations and get second order differential equations for $u_1(s)$ and $u_2(s)$:

$$\frac{d^2u_1(s)}{ds^2} + \frac{1}{2s}\frac{du_1(s)}{ds} + \frac{\alpha^2}{4}u_1(s) = \frac{\alpha}{4\sqrt{is}}I_1(s) - \frac{1}{2\sqrt{is}}\frac{dI_0(s)}{ds} \tag{63}$$

and

$$\frac{d^2u_2(s)}{ds^2} - \frac{1}{2s}\frac{du_2(s)}{ds} + \frac{\alpha^2}{4}u_2(s) = \frac{1}{4is}I_1(s) - \frac{i\alpha}{4}I_0(s) + \frac{i}{2}\frac{dI_1(s)}{ds}\,. \tag{64}$$

The solutions of these equations are elementary and easily obtained after some algebra as

$$u_1(s) = -\frac{\pi}{4\sqrt{2}}\int_{-\infty}^{\infty}dx'\psi(x',0)\left\{\int_0^s ds'\,\frac{s^{1/4}s'^{3/4}}{\sqrt{is'}}g_1(s,s')\right.$$
$$\left.\left[\alpha\,\mathrm{sgn}(x') + \frac{|x'|}{\sqrt{is'}}\right]e^{i\sqrt{is'}|x'|}\right\} \tag{65}$$

where

$$g_1(s,s') = J_{\frac{1}{4}}\left(\frac{\alpha s'}{2}\right)J_{-\frac{1}{4}}\left(\frac{\alpha s}{2}\right) - J_{\frac{1}{4}}\left(\frac{\alpha s}{2}\right)J_{-\frac{1}{4}}\left(\frac{\alpha s'}{2}\right)\,. \tag{66}$$

Here and in the following expressions $J_a(x)$, stands for the first kind of Bessel's function. The solution of the differential equation in Equation (64) is

$$u_2(s) = -\frac{\pi}{4\sqrt{2}}\int_{-\infty}^{\infty}dx'\psi(x',0)\left\{\int_0^s ds'\,s^{3/4}s'^{1/4}g_2(s,s')\right.$$
$$\left.\left[\frac{\mathrm{sgn}(x')}{is'} - i\alpha - \frac{ix'}{\sqrt{is'}}\right]e^{i\sqrt{is'}|x'|}\right\} \tag{67}$$

where

$$g_2(s,s') = J_{\frac{3}{4}}\left(\frac{\alpha s'}{2}\right)J_{-\frac{3}{4}}\left(\frac{\alpha s}{2}\right) - J_{\frac{3}{4}}\left(\frac{\alpha s}{2}\right)J_{-\frac{3}{4}}\left(\frac{\alpha s'}{2}\right)\,. \tag{68}$$

Note that

$$\mathcal{L}\left\{\frac{1}{t}\langle\psi(0,t)\rangle\right\} = u_1(s) = \int_s^{\infty}ds'\langle\bar{\psi}(0,s')\rangle \tag{69}$$

and

$$\mathcal{L}\left\{\frac{1}{t}\langle\psi_x(0,t)\rangle\right\} = u_2(s) = \int_s^{\infty}ds'\langle\bar{\psi}_x(0,s')\rangle\,. \tag{70}$$

Thus using Equations (69) and (70) in (41) we get

$$\bar{\psi}(x,s) = \int_{-\infty}^{\infty}dx'\psi(x',0)\left\{\frac{e^{i\sqrt{is}|x-x'|}}{2\sqrt{is}}e^{i\sqrt{is}|x-x'|}\right.$$
$$+\frac{\mathrm{sgn}(x)\,\pi\,\alpha\,s^{1/4}e^{i\sqrt{is}|x|}}{8\sqrt{2i}}\int_s^{\infty}ds's'^{1/4}g_1(s,s')\left[\alpha\,\mathrm{sgn}(x') + \frac{|x'|}{\sqrt{is'}}\right]$$
$$e^{i\sqrt{is'}|x'|} + \frac{\sqrt{i}\,\pi\,\alpha\,s^{1/4}\,e^{i\sqrt{is}|x|}}{8\sqrt{2}}\int_s^{\infty}ds's'^{1/4}g_2(s,s')$$
$$\left.\left[\frac{\mathrm{sgn}(x')}{is'} - i\alpha - \frac{ix'}{\sqrt{is'}}\right]e^{i\sqrt{is'}|x'|}\right\}\,. \tag{71}$$

Thus the Green's function in Laplace transformed space for the Schrödinger equation with a potential $V(x,t) = \frac{\alpha}{t}\delta'(x)$ is

$$G(x,x',s) = \left\{\frac{e^{i\sqrt{is}|x-x'|}}{2\sqrt{is}}e^{i\sqrt{is}|x-x'|} + \frac{\mathrm{sgn}(x)\,\pi\,\alpha\,s^{1/4}e^{i\sqrt{is}|x|}}{8\sqrt{2i}}\right.$$
$$\int_s^{\infty}ds's'^{1/4}g_1(s,s')\left[\alpha\,\mathrm{sgn}(x') + \frac{|x'|}{\sqrt{is'}}\right]e^{i\sqrt{is'}|x'|}$$
$$+\frac{\sqrt{i}\,\pi\,\alpha\,s^{1/4}\,e^{i\sqrt{is}|x|}}{8\sqrt{2}}\int_s^{\infty}ds's'^{1/4}g_2(s,s')$$
$$\left.\left[\frac{\mathrm{sgn}(x')}{is'} - i\alpha - \frac{ix'}{\sqrt{is'}}\right]e^{i\sqrt{is'}|x'|}\right\}\,. \tag{72}$$

This Green' s function cannot be converted in terms of elementary functions but it is possible to use numerical methods to obtain Green' s function in the position-time space.

4. CONCLUSION

In this work, we have studied some analytically solvable time-dependent point interactions. First, we have obtained a formal expression of the propagator for finite number of Dirac δ potentials with time dependent strengths and solved the time dependent Schrödinger equation for this system. Then we have investigated one δ potential with various time dependent strengths in more detail and found the propagator for N Dirac δ potential in the limit that centers are infinitely separated. Furthermore, we have found an expression of the propagator for finite number of δ' potentials with time dependent strengths and solved the time dependent Schrödinger equation for this potential. We believe that these results obtained are useful in models of ionization problems, where the particle is initially bound to the time dependent δ or δ' potentials. Such type of models have been studied (see e.g., [42, 51]) and the results obtained are compared with the experiment [52].

DATA AVAILABILITY STATEMENT

All datasets analyzed for this study are included in the article/**Supplementary Material**.

AUTHOR CONTRIBUTIONS

All authors listed have made a substantial, direct and intellectual contribution to the work, and approved it for publication.

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SUPPLEMENTARY MATERIAL

The Supplementary Material for this article can be found online at: https://www.frontiersin.org/articles/10.3389/fphy.2020.00065/full#supplementary-material

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Time Operators Determined by Cylindrical Processes

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The main purpose of this paper is to study time operators associated with cylindrical elements, i.e., generalized functions with values in locally convex spaces. It is given the characterization of the domains of the constructed time operators and partially resolved the problem of decomposability of random elements.

Keywords: time operator, pettis integral, absolutely summing operator, decomposability, cylindrical elements, cylindrical martingales

1. INTRODUCTION

The paper is devoted to extensions of internal time operators on the spaces of functions with values in topological vector spaces and on the spaces of generalized functions of this type associated with K-systems. The main reason of the introduction of time operators was the Lambda transformation theory formulated by I. Prigogine and his collaborators (see [1–3]) as a new approach to the theory of irreversibility in statistical physics. Precisely, to the problem of the relation between the reversible laws of dynamics and the observed irreversible (stochastic) evolution. Let us remind, that the classical view point was that irreversible behavior of the observed time evolution in a dynamical system can only arise from deterministic dynamics as the result of averaging (coarse-graining). The new approach can be formulated, in simplified terms, as a task to relate a given unitary evolution group $\{U_t\}_{t\in\mathbb{R}}$ acting on a Hilbert space of Gibbs' square integrable densities with an entropy increasing evolution semigroup $\{W_t\}_{t\in\mathbb{R}_+}$ through a similarity transformation called the transformation Λ (Lambda) (see [3]) as follows:

$$W_t\Lambda = \Lambda U_t, \quad t \in \mathbb{R}_+ . \tag{1}$$

Almost all known constructions of Λ transformations have been done so far for the dynamical systems which admit time operators (see [4] for another approach). Such dynamical systems allow the existence of Lyapunov variables, defined as functions of time operators, representing non-equilibrium entropy [1]. This is also a possible way to the task of defining time operator in quantum mechanics which in turn could allow to determine entropy operator. However, the class of dynamical systems for which time operators can be defined is very narrow, in fact, it is limited to K-systems.

Time operators were initially defined on the Hilbert space of square integrable functions. The problem of an extension of the concept of time operator was motivated by a need to extend the Λ transformation theory beyond square integrable probability densities. Indeed, it is natural to ask about a possibility to extend Λ and W_t on a larger class of states, including probability measures. Particularly interesting, from the physical point of view, is the possibility of extension on singular measures concentrated at single points of the phase space [2, 5–7].

Another motivation for the introduction and study of time operators is due to the recently discovered fact that time operators can be also associated with non-invertible dynamics and used as

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a new tool in the spectral analysis of evolution semigroups of unstable dynamical systems (see e.g., [8–13]). In this case time operators and evolution semigroups are defined on various topological vector spaces. The relation between the time operator T and the evolution semigroup $\{U_t\}$ is such that each U_t preserves the domain of T and satisfies the relation

$$TU_t = U_tT + tU_t\,. \tag{2}$$

The idea behind the spectral analysis of the evolution semigroup $\{U_t\}$ on a Hilbert space with the help of the time operator T is to decompose T in terms of a complete system of its eigenvectors $\{e_{n,k}\}$, $Te_{n,k} = ne_{n,k}$, such that $U_te_{n,k} = e_{n+t,k}$, as follows

$$T = \sum_n n \sum_k (\,\cdot\,, e_{n,k})e_{n,k}\,.$$

Similar spectral decompositions but in terms of Schauder bases or frames can be obtained in other topological vector spaces.

In this paper we will focus on the construction of time operators associated with K-systems acting on the spaces of cylindrical elements. A cylindrical element is an object which is a generalization of an E valued function, where E is a locally convex space. More precisely, p-cylindrical element, which will be defined in the next section, is a generalization of a weakly p-integrable function with values in E.

Although such extensions of time operators concern various topological vector spaces we will elaborate a unified approach based on the idea of stochastic integral with respect to cylindrical martingales (see [14]). We will also study the related problem of decomposability of cylindrical elements. It can happen that the action of a time operator or even a conditional expectation does not leave the space of vector valued functions invariant but leads to cylindrical elements instead. The decomposability of cylindrical elements allows to represent them again as measurable functions.

The paper is organized as follows. In section 2, we gathered the basic facts on cylindrical elements, cylindrical measures and cylindrical martingales. We focus on the Pettis integrability of vector valued functions and cylindrical elements. We also characterize vector spaces of Pettis integrable cylindrical elements. Section 3 is devoted to the construction of time operators with respect to cylindrical processes and to the solution of the problem of decomposability in two particular cases.

2. CYLINDRICAL ELEMENTS AND CYLINDRICAL MARTINGALES

Throughout this paper, by a locally convex space (l.c.s.) or a topological vector space (t.v.s) we mean a Hausdorff l.c.s. (respectively t.v.s.) not equal to $\{0\}$ over the field of real or complex scalars. If E is an l.c.s. then E' denotes its topological dual and $\langle x, x'\rangle$ stands for the value of a functional $x' \in E'$ at $x \in E$. For subsets $A \subset E$ and $B \subset E'$ the symbols A° and B° denote the polars with respect to the duality $\langle E, E'\rangle$ and $\langle E', E\rangle$ respectively, i.e., $A^\circ = \{x' \in E' : |\langle x, x'\rangle| \leq 1,\ \text{for each } x \in A\}$ and $B^\circ = \{x \in E : |\langle x, x'\rangle| \leq 1,\ \text{for each } x' \in B\}$. By $\sigma(E', E)$ we shall denote the weak topology on E' and by $\tau(E', E)$ the Mackey topology, i.e., is the topology of uniform convergence on all $\sigma(E, E')$–compact, convex, circled subsets of E. E'_τ will denote the space E' with the Mackey topology. An l.c.s. E is quasi-complete if each bounded closed subset of E is complete.

Let $(\Omega, \mathcal{A}, P)$ be a probability space, $L^p = L^p(\Omega, \mathcal{A}, P)$, $p \geq 0$, and let E be an l.c.s.. By a *p-cylindrical element*, or simply *cylindrical element*, we mean a linear operator $X : E' \to L^p$. Notice that any function $x(\cdot) : \Omega \to E$ such that $\langle x(\cdot), x'\rangle \in L^p$ determines the cylindrical element

$$Xx' = X_{x(\cdot)}x' = \langle x(\cdot), x'\rangle\,.$$

Let us now introduce the concept of Pettis integrability of cylindrical elements. The reason of doing this is the following. In statistical physics the main object of interest is the time evolution of statistical ensembles, represented mathematically as probability distributions. However, for technical reasons we often take only some classes of probability distributions as the states of the system. In our case we confine to those probability measures which are absolutely continuous with respect to some reference measure. This allows to replace measures by their densities (Radon-Nikodyn derivatives) or by classes of integrable functions in general. Nevertheless, for a given integrable function f we can recover the corresponding measure μ_f putting

$$\mu_f(A) = \int_A f\,dP\,, \quad A \in \mathcal{A}\,. \tag{3}$$

Replacing f by a vector valued function $\vec{f} : \Omega \to E$ we should be able to recover the corresponding measure $\mu_{\vec{f}}$ like in (3) but this is not always possible. For example, if E is a Banach space and $\vec{f}$ a measurable function such that $\|\vec{f}\|$ is integrable then (3) holds and defines E-valued measure. However this is not true, in general, under the weaker assumption of integrability of $|\langle\vec{f}, x'\rangle|$, for all $x' \in E$. Additional assumptions have to be imposed on $\vec{f}$ such as the Pettis integrability defined below. The same can happen when we replace vector valued functions by cylindrical elements.

We say that a cylindrical element $X : E' \to L^0$ is *Pettis integrable* if $X(E') \subset L^1$ and for each $A \in \mathcal{A}$ there exists $x_A \in E$ such that

$$\langle x_A, x'\rangle = \int_A Xx'\,dP \quad \text{for each } x' \in E'\,. \tag{4}$$

We write

$$\int_A X\,dP = x_A\,. \tag{5}$$

and call it the *Pettis integral* of the cylindrical element X. Replacing in (4) and (5) X by a vector valued function $\vec{f}$ we obtain the classical definition of the Pettis integral (see [15]).

General properties of Pettis integrable cylindrical elements are in ref. ([16]). Here we will show relations between Pettis integrability and continuity of cylindrical elements.

We have

Proposition 1. ([16, 17]) Let E be a sequentially complete l.c.s. space and $X : E' \to L^1$ a cylindrical element. Then the following conditions are equivalent

(1) T is Pettis integrable

(2) T is $(\tau(E', E), \|\cdot\|_{L^1})$ continuous.

Actually, the implication (2) $\Rightarrow$ (1) in the above Proposition is valid without the assumption of sequential completeness (see [17]).

Let us also mention about two properties of Pettis integrable cylindrical elements which will be used later:

Proposition 2. If E and F are l.c.s., $S : E \to F$ is a continuous linear operator and $X : E' \to L^1$ is a Pettis integrable cylindrical element, then the linear operator $X \circ S^* : F' \to L^1$ is Pettis integrable and

$$S\left(\int_A X\, dP\right) = \int_A X \circ S^*, \quad \text{for each } A \in \mathcal{A}.$$

Proposition 3. If X is a Pettis integrable cylindrical element then for each absolutely convex neighborhood of 0 in E

$$\sup_{x' \in U^\circ} \int_\Omega |Xx'|\, dP < \infty$$

The proofs of the above properties can be found in [17].

It follows from Proposition 3 that if E is a normed space then X is a bounded linear operator form E' to L^1 with the operator norm

$$\|X\| = \sup_{\|x'\| \le 1} \int_\Omega |Xx'|\, dP$$

Notice that $\sigma(L^1, L^\infty)$ compactness of a family of functions in L^1 is equivalent to its uniform integrability (Dunford-Pettis Theorem) thus using the Vallèe-Poussin Theorem (see e.g., [18]) we obtain

Corollary. If $p > 1$, E is a reflexive Banach space and $X : E' \to L^p$ a continuous cylindrical element then X is Pettis integrable.

Let E be an l.c.s. and let $\mathcal{L}^p(E)$, $p \ge 1$, denote the space of all separably valued and weakly p-integrable functions $x(\cdot) : \Omega \to E$ with the topology generated by the family of seminorms

$$|||x(\cdot)|||_{U^\circ} = \sup_{x' \in U^\circ} \int_\Omega |\langle x(\cdot), x'\rangle|^p\, dP < \infty,$$

where U are convex and circled neighborhoods of zero in E.

It follows from ([16], Prop. 3.2, Th. 3.1 and Th. 3.2) that if E is a locally convex Fréchet space and $p = 1$ then the completion $\widehat{\mathcal{L}}^1(E)$ consists of all cylindrical elements $X : E' \to L^1$ which are $(\tau(E', E), \|\cdot\|_{L^1})$ continuous and compact linear maps. In general, we will denote by $\widehat{\mathcal{L}}^p(E)$ the completion of $\mathcal{L}^p(E)$.

If $X \in \widehat{\mathcal{L}}^p$ then for each fixed $g \in L^q$, $\frac{1}{p} + \frac{1}{q} = 1$, the map

$$x' \longmapsto gXx'$$

from E' to L^1 is a Pettis integrable cylindrical element.

Let us also recall some relations between cylindrical elements and cylindrical measures on a locally convex space E. Denote by $\mathcal{C}(E)$ the σ-field generated by cylindrical sets in E, i.e., the sets of the form

$$\{x \in E : (\langle x, x'_1\rangle, \ldots, \langle x, x'_n\rangle) \in B\},$$

where $n \in \mathbb{N}$, $x'_1, \ldots, x'_n \in E'$, $B \in \mathcal{B}_{\mathbb{R}^n}$ ($\mathcal{B}_{\mathbb{R}^n}$ denotes the Borel σ-field in $\mathbb{R}^n$).

Let μ be a finitely additive measure on $\mathcal{C}(E)$ and let

$$\mu_{x'_1,\ldots,x'_n}(B) \stackrel{\text{df}}{=} \mu\{x \in E : (\langle x, x'_1\rangle, \ldots, \langle x, x'_n\rangle) \in B\}.$$

The measure μ is called *cylindrical* if for each $n \in \mathbb{N}$ and $x'_1, \ldots, x'_n \in E'$ $\mu_{x'_1,\ldots,x'_n}$ is a probability measure on $(\mathbb{R}^n, \mathcal{B}_{\mathbb{R}^n})$.

Each cylindrical element X determines a cylindrical measure μ defined as

$$\mu(\{x \in E : (\langle x, x'_1\rangle, \ldots, \langle x, x'_n\rangle) \in B\}) = P\{(Xx'_1, \ldots, Xx'_n) \in B\}.$$

Conversely, if μ is a cylindrical measure on $\mathcal{C}(E)$ then there exist a probability space $(\Omega, \mathcal{A}, P)$ and a cylindrical element $X : E' \to L^0(\Omega, \mathcal{A}, P)$ satisfying the above equality (see [19]). The correspondence between cylindrical measures and cylindrical elements is one-to-one.

If μ is a cylindrical measure and X_μ the corresponding cylindrical element such that

$$\int_\Omega |X_\mu x'|^p\, d\mu < \infty, \quad \text{for each } x' \in E',$$

and some $p > 0$, then we say that μ has a *weak p-order*.

An important property of a cylindrical measure is its concentration on some families of sets. Namely, let $\mathfrak{S}$ be a family of subsets of E and μ a cylindrical measure on $\mathcal{C}(E)$. We say that μ is scalarly concentrated on $\mathfrak{S}$ if for each $\varepsilon > 0$ there is $A \in \mathfrak{S}$ such that

$$(\mu_{x'})_*(x'(A)) \ge 1 - \varepsilon,$$

for each $x' \in E'$, where $*$ denotes the inner measure.

Assume that $\mathfrak{S}$ is the family of all compact circled subsets of E and denote by $E'_{\mathfrak{S}}$ the space E' with the topology of uniform convergence on the sets from $\mathfrak{S}$. One of the basic relations between Pettis integrable cylindrical elements and the corresponding cylindrical measures is contained in the following Proposition.

Proposition 4. Let E be a complete l.c.s., $\mathfrak{S}$ the family of all compact circled subsets of E and X a cylindrical element. If $X \in \widehat{\mathcal{L}}^p(E)$, $p \ge 1$, then the corresponding cylindrical measure μ is scalarly concentrated on $\mathfrak{S}$.

The proof of this Proposition is based on the fact that X is $(\tau(E', E), \|\cdot\|_{L^p})$ continuous cylindrical element from E' to L^p which transforms equicontinuous subsets of E' into relatively compact sets in L^p, $p > 1$ (see also the proof of Th.4.1 in [16]).

The converse implication is not true in general even for Radon measures but is true for cylindrical Gaussian measures and corresponding L^2–valued cylindrical elements (see [16] for details).

3. TIME OPERATOR

Before defining time operator acting on cylindrical elements let us remind the classical construction which is based on the idea of Misra-Prigogine-Courbage [3]. Let us consider an abstract dynamical system given by the quadruple $(\Omega, \mathcal{A}, \mu, \{S_t\})$, where $\{S_t\}$ is a group of one-to-one μ invariant transformations of Ω and either $t \in \mathbb{Z}$ or $t \in \mathbb{R}$.

A *K-flow* (we will say *K-system*) is a probability space $(\Omega, \mathcal{A}, P)$ with a group of measure preserving transformations S_t, $t \in \mathbb{R}$, of Ω. We assume that there exists a σ-algebra $\mathcal{A}_0 \subset \mathcal{A}$ such that the family $\{\mathcal{A}_t\}_{t\in\mathbb{R}}$, $\mathcal{A}_t \stackrel{\text{df}}{=} S_t(\mathcal{A}_0)$ has the properties

(i) $\mathcal{A}_s \subset \mathcal{A}_t$, for $s < t$
(ii) $\sigma\left(\bigcup_{t\in\mathbb{R}} \mathcal{A}_t\right) = \mathcal{A}$
(iii) $\bigcap_{t\in\mathbb{R}} \mathcal{A}_t = \mathcal{A}_{-\infty}$ – the trivial σ-algebra, i.e., the algebra of sets of measure 0 or 1.

where $\sigma\left(\cup_{t\in\mathbb{R}}\mathcal{A}_t\right)$ stands for σ-algebra generated by $\mathcal{A}_t$, $t \in \mathbb{R}$.

We replace deterministic evolution of phase space points by the Liouville evolution of probability density functions putting

$$U_t\, \rho(\omega) = \rho(S_{-t}\omega)\,, \tag{6}$$

where ρ is $\mathcal{A}$ measurable function on Ω. The invariance of the measure μ implies that the transformations U_t considered as operators on $L^2 = L^2(\Omega, \mathcal{A}, \mu)$ form a unitary group.

In this setting a possible approach to the problem of irreversibility can be formulated as in section 1. Namely it is constructed the Lambda operator connecting the reversible group $\{U_t\}_{t\in\mathbb{R}}$ with an entropy increasing evolution semigroup $\{W_t\}_{t\geq 0}$. It is assumed that Λ is a bounded linear operator on $L^2(\Omega, \mathcal{A}, \mu)$ with densely defined inverse Λ^{-1} such that $W_t = \Lambda U_t \Lambda^{-1}$ defines, for $t \geq 0$, a continuous one-parameter group of contractions. For physical reasons it is also additionally assumed that Λ is positivity preserving, $\Lambda 1 = 1$ and $\|W_t(\rho - 1)\|$ decreases strictly monotonically to 0, as $t \to +\infty$, for all densities $\rho \not\equiv 1$. The last condition means that the entropy of the system tends strictly monotonically to zero when the system approaches equilibrium.

In classical dynamical systems Lambda transformations have been constructed on the L^p spaces associated with K-systems as functions of time operators. The main idea of such construction is ([3] see also [20–22]) that each K-system determines the family $\{\mathbf{E}_t\}_{t\in\mathbb{R}}$ of conditional expectations,

$$\mathbf{E}_t = \mathbf{E}^{\mathcal{A}_t}\,,$$

which in turn defines the operator T on each space $L^p = L^p(\Omega, \mathcal{A}, P)$, $p \geq 1$,

$$T = \int_{-\infty}^{+\infty} t d\mathbf{E}_t\,, \tag{7}$$

which is called the *time operator*.

In the case of discrete time, $t \in \mathbb{Z}$, we consider the group $\{S_n\}_{n\in\mathbb{Z}}$ generated by a single measure preserving transformation S, i.e., $S_n = S^n$, for $n \neq 0$, and $S^0 = I$. The time operator T is then defined as

$$T = \sum_{n=-\infty}^{\infty} nE_n\,.$$

If $p = 2$ then the above integral, or sum, defining T is just the spectral resolution of a selfadjoint operator. In this case $\{U_t\}_{t\in\mathbb{R}}$ defined in (6) is a unitary group on L^2 satisfying the following relation with T

$$U_t T U_{-t} = T + tI\,, \tag{8}$$

which is equivalent to (2).

The transformation Λ is defined, up to constants, as an operator function $\Lambda = \Lambda(T)$. Namely

$$\Lambda = f(T) + E_{-\infty}$$

where $E_{-\infty}$ is the projection on the space $L^2(\mathcal{A}_{-\infty}) = \mathbb{R}$. The function f is assumed to be positive, decreasing on $\mathbb{R}$, $f(-\infty) = 1, f(+\infty) = 0$ and such that $\ln f$ is concave on $\mathbb{R}$. Then, for any such function f the corresponding operator Λ is injective on L^2, one-to-one with densely defined inverse (see ref. [21]). Moreover the semigroup

$$W_t \stackrel{\text{df}}{=} \Lambda U_t \Lambda^{-1}\,,\ \ t \geq 0\,, \tag{9}$$

is Markovian and $\|W_t p - 1\|_{L^2}$ decreases to 0, for each density $\rho \neq 1$ and together with $\{U_t\}$ satisfies the relation (1).

The time operator as defined in (7) uses the family of conditional expectations $\{\mathbf{E}_t\}$ which can be treated as a spectral family of projectors on the Hilbert space L^2 which defines a selfadjoint operator or, for a given $\rho \in L^2$, $\{\mathbf{E}_t\rho\}$ can be considered as a martingale with respect to the filtration $\{\mathcal{A}_t\}$. In the latter case the integral defining T can be understood as a stochastic integral with respect to a martingale. Such approach allows to define time operators on larger classes of function, for example on L^1. Moreover the stochastic integral technique allows to replace the family of projectors $\{\mathbf{E}_t\}$ by a family of operators $\{M_t\}$ such that for a given ρ $\{M_t\rho\}$ is a martingale with respect to $\{\mathcal{A}_t\}$. In fact, such a generalization of the definition of time operators has been proposed in [22]. The extension of the definition of T on L^1 spaces can be found in [23].

It should be stressed that the above mentioned extension of the time operator concerns such states (probability measures) which have densities. However, in statistical physics the class of states can be larger and contain, for example, singular measures. There were successful attempts of such extension of the domain of time operators (see [2, 5, 6]).

We will define now a time operator acting on p-cylindrical elements. As we have seen in section 2 p-cylindrical element is actually a generalization of a weakly p-integrable function with values in a topological vector space. Equivalently, time operators will act on cylindrical measures on a topological vector spaces. This is a significant step beyond the classical L^p space.

We have to define first the conditional expectation of a cylindrical element. Let $\mathbf{E}^{\mathcal{B}} : L^1(\mathcal{A}) \to L^1(\mathcal{B})$ denote the usual

operator of the conditional expectation (see [18]), and let $Y : E'_\tau \to L^p$, $p \geq 1$, be a p-cylindrical element obtained as the composition of operators $\mathbf{E}^{\mathcal{B}}$ and X. Note that if $X : E'_\tau \to L^p$ is continuous, then $Y = \mathbf{E}^{\mathcal{B}}X$ is also continuous. Thus, if $X : E'_\tau \to L^p$ is continuous, $1 \leq p < \infty$, then for each sub σ-field $\mathcal{B} \subset \mathcal{A}$ the 1-cylindrical element $Y = \mathbf{E}^{\mathcal{B}}X : E'_\tau \to L^1$ satisfies

$$\int_B Y dP = \int_B \mathbf{E}^{\mathcal{B}} X dP = \int_B X dP\,,$$

for each $B \in \mathcal{B}$.

The above definition of conditional expectation applies, in particular, to Banach space valued functions. Indeed, each function $x(\cdot) : \Omega \to E$, where E is a Banach space, which has a weak p-order defines a cylindrical element $X : E'_\tau \to L^p$. Thus we can define the conditional expectation of $x(\cdot)$

$$\mathbf{E}^{\mathcal{B}} x(\cdot) = \mathbf{E}^{\mathcal{B}} X\,.$$

It should be noticed that it is not always possible to define the conditional expectation of a Banach space valued function which is not strongly integrable. Indeed one can find (see [24]) a Pettis integrable function $x(\cdot)$ with values in a reflexive Banach space E and a sub σ-algebra $\mathcal{B}$ for which does not exist any $\mathcal{B}$ measurable function $y(\cdot) : \Omega \to E$ such that

$$\int_B \langle y(\cdot), x'\rangle dP = \int_B \langle x(\cdot), x'\rangle dP\,, \quad \text{for } B \in \mathcal{B}\,,\ x' \in E'\,.$$

However, we have shown above that this conditional expectation exists as a cylindrical element although not generated by a measurable function. Thus the replacement of Pettis integrable functions by the corresponding cylindrical elements allows to give a meaning to a generalization of the concept of conditional expectation.

Let us assume that E is a complete l.c.s. and $\mathcal{I}$ a linear ordered set. A family $\{X_t\}_{t\in\mathcal{I}}$ of cylindrical elements $X_t : E' \to L^p$, $t \in \mathcal{I}$, will be called the p-cylindrical process. If each X_t is Pettis integrable then the process will be also called Pettis integrable. Recall that Pettis integrability is equivalent $(\tau(E', E), \|\cdot\|_{L^1})$ continuity - Proposition 1.

Let $\{\mathcal{B}_t\}_{t\in\mathcal{I}}$ be a family of σ-fields such that $\mathcal{B}_t \subset \mathcal{A}$ and $\mathcal{B}_{t_1} \subset \mathcal{B}_{t_2}$, for $t_1 < t_2$. A p-cylindrical process $\{X_t\}_{t\in\mathcal{I}}$, where $p \geq 1$, is called p-cylindrical martingale if it is adapted with respect to $\{\mathcal{B}_t\}_{t\in\mathcal{I}}$, each X_t is $(\tau(E', E), \|\cdot\|_{L^p})$ continuous, and $\mathbf{E}^{\mathcal{B}_s} X_t = X_s$, for $s < t$.

It is easy to show that a τ-continuous p-cylindrical process $\{X_t\}_{t\in\mathcal{I}}$ is p-cylindrical martingale if and only if $\{X_t x'\}_{t\in\mathcal{I}}$ is a real martingale for each $x' \in E'$. The proposition below shows that for cylindrical martingales we have an analog of the classical convergence theorem (see [25]).

Proposition 5. Let $\{X_t x'\}_{t\in\mathcal{I}}$ be a discrete time p-cylindrical martingale with respect to $\{\mathcal{B}_t\}_{t\in\mathcal{I}}$, $p > 1$, and assume that E'_τ is barreled Barreled space. If

$$\sup_{t\in\mathcal{I}} \mathbf{E}|X_t x'|^p < \infty\,, \quad \text{for each } x' \in E'\,,$$

then there exists a continuous cylindrical element $X : E'_\tau \to L^p$ such that

$$X_t = \mathbf{E}^{\mathcal{B}_t} X\,, \quad \text{for each } t \in \mathcal{I}\,,$$

and X_t converges to X in L^p norm.

This proposition is not true in the case $p = 1$. However assuming that

$$\mathbf{E} \sup_t |X_t x'| < \infty\,, \quad \text{for each } x' \in E'\,, \tag{10}$$

we obtain an analog of Proposition 5.

In the case of continuous time we can obtain similar results under the additional assumption of right continuity of the considered martingales. The assumption of right continuity of a martingale $\{m_t\}$ allows to define the stochastic integral $\int f(t)\, dm_t$, where $f(t)$ is a Borel measurable function (see [26]).

The object of our interest will be the cylindrical martingales generated by a single cylindrical element, like in the thesis of Proposition 5, associated with the filtration $\{\mathcal{B}_t\}_{t\in\mathbb{R}}$ determined by a given. K-flow.

Let $\{\mathcal{A}_t\}$ be a family of σ-algebras of a given K-flow and $\{M_t\}$ an associated operator valued martingale i.e., a family of bounded operators on L^p, $p \geq 1$, such that $\{M_t\}$ is a right continuous martingale with respect to $\{\mathcal{A}_t\}$. In the classical approach (see [22] for the details) it was assumed that $\{M_t\}$ acts on L^2, has orthogonal increments: for $s_1 \leq s_2 < t_1 \leq t_2$ $(M_{s_2} - M_{s_1})(M_{t_2} - M_{t_1}) = 0$ and that M_∞ is a positive one-to-one operator satisfying

$$M_\infty 1 = 1 \quad M_\infty U_t = U_t M_\infty \quad \text{for each } t \in \mathbb{R}\,,$$

where U_t is given by (6). It was shown that for a fixed monotonic function f on $\mathbb{R}$ the transformation

$$\rho \mapsto \int f(t)\, dM_t \rho + M_{-\infty}\rho\,, \quad \rho \in L^2\,. \tag{11}$$

is well-defined on the domain D_f which is dense in L^2. Taking $f(t) = t$ we obtain the time operator. If we assume that f is a positive non-increasing function on $\mathbb{R}$ with $\lim_{t\to-\infty} f(t) = 1$, $\lim_{t\to\infty} f(t) = 0$ and such that for each $t \in \mathbb{R}$ the quotient $f(s)/f(s - t)$ is a bounded and non-increasing function of s then (11) defines the discussed above similarity transformation Λ which in turn defines the Markov semigroup (9).

Note that taking $M_t = \mathbf{E}_t$, where $\mathbf{E}_t = \mathbf{E}^{\mathcal{A}_t}$, we obtain an operator valued martingale satisfying the required properties. Moreover, a cylindrical element X with values in L^p defines the p-cylindrical martingale $\{\mathbf{E}_t X\}$. Therefore, in the case $p = 2$ we can apply directly the above construction putting in (11) Xx', $x' \in E'$, instead of ρ. Replacing the space L^2 by $L^2 \ominus 1$ we can omit the second component in (11) obtaining the following operator $f(\mathbf{T})$ acting on cylindrical elements

$$f(\mathbf{T})(X) = \int f(t)\, d\mathbf{E}_t X\,. \tag{12}$$

We can not apply directly the above approach in the case $p \geq 1$, $p \neq 2$. Here we have to use a different approach to stochastic

integration. The theory of integrals $\int f(t)\,dm_t$, where $\{m_t\}$ is a p-integrable martingale can be found in Bichteler's paper [26]. This integral is defined first for simple functions (or processes) $f(t)$. Then it is said that $\{m_t\}$ is an L^p-integrator if $\{m_t\}$ is p-integrable and the linear operator $f \mapsto \int f(t)\,dm_t$ from the space of elementary integrands to L^p has an extension satisfying the dominated convergence theorem (see Def.1 in [26]).

Theorem 1. Let E be an l.c.s. and $(\Omega, \mathcal{A}, \mu, \{S_t\})$ a K-flow. If $1 < p < \infty$ then for any simple function f with a bounded support the linear operator on $L(E', L^p)$

$$f(\mathbf{T})(X) = \int f(t)\,d\mathbf{E}_t X\,.$$

is correctly defined, for each $x' \in E'$, the martingale $\{\mathbf{E}_t Xx'\}$ is an L^p-integrator and we have

$$\left\| \int f(t)\,d\mathbf{E}_t Xx' \right\|_{L^p} \leq C_p \|\mathbf{E}_\tau Xx'\|_{L^p}\,,$$

where τ is such that $f(t) = 0$, for $|t| > \tau$ and C_p is a constant which depends only on p.

If $p = 1$ then the above integral exists and the martingale $\{\mathbf{E}_t Xx'\}$ is an L^1-integrator under the additional assumption that

$$\mathbf{E}(|Xx'| \log |Xx'|) < \infty\,, \quad \text{for each } x' \in E'\,, \tag{13}$$

Proof. If $p > 1$ we can apply (3.8) from [26] which says that a p-intergrable martingale is an L^p-integrator. If $p = 1$ we use Th. 7.2 from [26] and the additional assumption (13) to show that for each $x' \in E$" the martingale $\{\mathbf{E}_t Xx'\}$ is an L^1 integrator. Note that because the martingales satisfy the assumption (13), in the latter case, they are elements of the Hardy space H^1, i.e., (10) is satisfied.

It follows from Theorem 1 that $f(\mathbf{T})$ can be defined for simple functions with bounded support. However, because of the dominated convergence theorem we can extend the class of functions taking, for example, $f(t) = t$ to obtain the operator

$$\mathbf{T} = \int t\,d\mathbf{E}_t\,,$$

which acts on the space $L(E', L^p)$.

Let $\{\mathbf{U}_t\}$ be the evolution group on $L(E', L^p)$ associated with the transformations $\{S_t\}$, i.e., for $X \in L(E', L^p)$, $\mathbf{U}_t X$ is a cylindrical element of the form

$$(\mathbf{U}_t X)x'(\omega) = Xx'(S_{-t}\omega)\,.$$

Using the relation $\mathbf{E}_{s+t}U_t = U_t\mathbf{E}_s$ valid for conditional expectations associated with the K-system and the evolution $\{S_t\}$ on the ordinary L^p-space (see e.g., [21]) we obtain that also

$$\mathbf{E}_{s+t}\mathbf{U}_t = \mathbf{U}_t\mathbf{E}_s\,.$$

This leads to the following

Corollary. The operator $\mathbf{T}$ is a time operator on the space $L(E', L^p)$ associated with the evolution $\{\mathbf{U}_t\}$.

We can also take as f a bounded monotonic function with the listed above properties to obtain an analog of the operator Lambda, $\Lambda = f(\mathbf{T})$. An important example of applications the above construction of $\mathbf{T}$ is the possibility to define time operators on the spaces of weakly integrable E-valued functions. This is because the constructed above stochastic integral transforms cylindrical elements into cylindrical elements. If we take as an argument of $\mathbf{T}$ the cylindrical element generated by an E valued function then after the transformation it need not to remain a function (see remarks concerning the conditional expectation of Pettis integrable functions). However $f(\mathbf{T})$ leaves the space $L(E', L^p)$ invariant.

An important question is: When a cylindrical element is generated by a measurable function defined on Ω with values in the vector space E? Similar question concerns martingales: When the integral transformation of a p-cylindrical martingale generated by a vector valued function will be still a function generated martingale? The rest of this section is devoted to an answer to these questions.

Let us introduce first the following definition:

We say that X is p-decomposable, $p > 0$, if there exists a measurable function $x(\cdot) : \Omega \to E$ such that

1^0 $Xx' = \langle x(\cdot), x'\rangle$, for each $x' \in E'$

2^0 $\int_\Omega \|x(\cdot)\|^p\,dP < \infty$, for each continuous seminorm $\|\cdot\|$ on E.

Decomposability of a cylindrical element depends both on properties of X as a linear operator and on the topological properties of the vector space E. We will consider the problem of decomposability in both cases. We begin with the dependence of the decomposability of a cylindrical element $X : E' \to L^1$ on the properties of E. It is obvious that if E is finite dimensional then each 1-cylindrical element is 1-decomposable. If E is infinite dimensional then the space $\mathcal{L}^1(E)$ of Pettis integrable functions on Ω with values in E, introduced in section 2, is not complete in general and its completion $\widehat{\mathcal{L}^1}(E)$ may contain cylindrical elements which are not associated with any measurable function. However, the transformations like conditional expectation or time operator leave $\widehat{\mathcal{L}^1}(E)$ invariant. Thus we can ask if there are locally convex spaces for which this completion remains a function space. The next theorem shows such a possibility.

Theorem 2. Let E be a locally convex nuclear Fréchet space. Then each element of $\widehat{\mathcal{L}^1}(E)$ is 1-decomposable.

Proof. In the proof we will use some results concerning tensor products of l.c.s.. Let us first introduce the notation and remind the relevant facts (see [27]). Let E be an l.c.s., F a Banach space and $E \otimes F$ the algebraic tensor product. We define two basic topologies on $E \otimes F$. First is the ε-topology generated by the seminorms

$$\varepsilon_U(z) = \sup_{x' \in U^\circ} \sup_{y' \in B^\circ} |\langle z, x' \otimes y'\rangle|\,, \quad \text{for } z \in E \otimes F\,,$$

where U runs over a basis of convex and circled neighborhoods of 0 in E and B is the unit ball in F. By $E\hat{\otimes}_\varepsilon F$ we denote the completion of $E \otimes F$ in the ε-topology.

The second topology, called the projective topology, is generated by the seminorms

$$\pi_U(z) = \inf \sum_i p_U(x_i)\|y_i\|$$

where the infinitum is taken over all representations of the element $z = \sum_{i=1}^{n} x_i \otimes y_i$ and U is an absolutely convex neighborhood of 0 in E. By $E\hat{\otimes}_\pi F$ we denote the completion of $E \otimes F$ in the projective topology.

Note that the ε-topology and the projective topology are respectively the weakest and the strongest topology on the tensor product of two l.c.s. which are generated by cross-seminorms (see [27]).

It is known that if E is a Banach space then $E\hat{\otimes}_\pi L^1$ is norm isomorphic to the space $L^1(E)$ of all E valued Bochner integrable functions f on Ω endowed with the norm $\|f\|_{L^1(E)} = \int_\Omega \|f(\omega)\|\, P(d\omega)$. If E is just an l.c.s. then $E\hat{\otimes}_\pi L^1$ is isomorphic with $L^1(E)$ defined as the space of all strongly measurable functions f such that $\|f(\cdot)\|$ is integrable for each semi-norm $\|\cdot\|$ on E.

We have shown in [16] that if E is a separable l.c.s. Fréchet space then $\widehat{\mathcal{L}}^1(E)$ can be identified (is isomorhic) with $E\hat{\otimes}_\varepsilon L^1$. However, when E is a complete nuclear l.c.s. the latter space is isomorphic to $E\hat{\otimes}_\pi L^1$ (see [27]). Therefore, each element from $\widehat{\mathcal{L}}^1(E)$ is represented by a Bochner integrable function which ends the proof.

It follows from the above theorem that for a nuclear space valued functions the Pettis integrability is equivalent to the Bochner integrability like in the finite dimensional case.

Let now consider the dependence between decomposability and operator properties of cylindrical elements. It is known that if $E = H$ – is a Hilbert space then a 2-cylindrical martingale $X : H' \to L^2$ is 2-decomposable if and only if the mapping

$$H' \ni h \mapsto X_t h \in L^2$$

is a Hilbert-Schmidt operator for any t (see [14]).

We can also decompose cylindrical elements by composing them with Hilbert-Schmidt operators or, more generally, with absolutely summing operators. The problem of decomposability of a cylindrical element acting on a Banach space through a composition with an absolutely summing operator has been already resolved (see [25, 28] and references therein). Here, we will resolve this problem in the case of cylindrical elements acting on locally convex spaces.

If E and F are normed spaces and $0 < p < \infty$ then a linear operator $S : E \to F$ is said to be p-absolutely summing if there exists a constant C such that for each $x_1, \ldots, x_n \in E$

$$\sum_{i=1}^{n} \|Sx_i\|^p \le C \sup_{\|x'\| \le 1} \sum_{i=1}^{n} |\langle x_i, x' \rangle|^p .$$

In the sequel we will use the following Pietsch Majorization Theorem:

Proposition 6. ([29], p. 232) Let E and F be normed spaces. An operator $S : E \to F$ is p-absolutely summing, $0 < p < \infty$, if there exist a constant C and a Radon probability measure μ on the unit ball U° of E', where U° is equipped with the $\sigma(E', E)$ - topology, such that

$$\|Sx\|^p \le C \int_{U^\circ} |\langle x, x' \rangle|^p \, d\mu(x') \text{ for all } x \in E .$$

We shall now extend the definition of the p-absolutely summing operatoron operators acting on an l.c.s. with values in a t.v.s.. Consider first the case of an operator $S : E \to F$, where F is a quasi-normed space. Recall that a quasi-norm on F is a non-negative positively defined homogenous function $\|\cdot\|$ such that for some r, $0 < r \le 1$, we have

$$\|x + y\|^r \le \|x\|^r + \|y\|^r , \quad x, y \in E .$$

We then say that the space F is r-normed.

Remark:

(i) An r-normed space is s-normed for $0 < s \le r \le 1$
(ii) If $0 < r \le 1$ then the space L^r is r-normed.

The definition of a p-absolutely summing operator $S : E \to F$, for E normed and F quasi-normed space, is the same as in the case of normed spaces. Moreover, the Proposition 6 remains true and we have

Proposition 7. ([29]) Let Ω be a compact Hausdorff space and ν a probability measure on Ω. Then the canonical embedding of the space $C(\Omega)$ (continuous functions on Ω) into $L^p(\Omega, \nu)$ is p-absolutely summing for $0 < p < \infty$.

Before we turn to the further generalization of the concept of p-absolutely summing operators we shall introduce first some auxiliary normed spaces and decompositions of bounded operators on topological vector spaces.

Let E be an l.c.s. and U an absolutely convex neighborhood of 0 in E. By E_U we denote the normed space $\left(E/p_U^{-1}(\{0\}), p_U(\cdot)\right)$ where $p_U(\cdot)$ is the Minkowski functional of U. Let $\hat{E}_U$ denotes the completion of E_U in the norm $p_U(\cdot)$ and Φ_U the canonical map from E into E_U (or into $\hat{E}_U$). Of course Φ_U is continuous. Now, let F be a t.v.s.. A subset B of F is said to be p-absolutely convex if whenever it contains x and y it contains all $\alpha x + \beta y$ with $|\alpha|^p + |\beta|^p \le 1$. If $p = 1$ then B is absolutely convex. We put

$$\|x\|_B = \inf\{\lambda > 0 : x \in \lambda B\} ,$$

and $F_B = \bigcup_{n=1}^{\infty} nB$. Then $(F_B, \|\cdot\|_B)$ is p-normed and the canonical injection
$\Psi_B : F_B \to F$ is continuous. Moreover, F_B is complete if B is complete.

A subset B of F is called quasi-absolutely convex if it is p-absolutely convex for some $0 < p \le 1$.

Let E be an l.c.s., F be a t.v.s. and $S : E \to F$ a bounded linear operator, i.e., such that there exists a neighborhood U of 0 in E for which $S(U)$ is bounded. Then S can be decomposed in the following way

$$\begin{array}{ccc} E & \xrightarrow{S} & F \\ {\scriptstyle \Phi_U}\downarrow & & \uparrow{\scriptstyle \Psi_B} \\ E_U & \xrightarrow[S_0]{} & F_B \end{array}$$

where U is an absolutely convex neighborhood of 0 in E and B is a bounded subset of F. If B can be chosen quasi-absolutely

convex, then S_0 is a continuous linear operator from the normed space E_U into the quasi-normed space F_B. Moreover, if B is complete then S_0 has the continuous extension $\bar{S}_0$ from the Banach space $\hat{E}_U$ into F_B. Note that if F is an l.c.s. then F_B is a normed space.

We can now define p-absolutely summing operator on a locally convex space. Let E be an l.c.s. and F be a t.v.s.. A linear operator $S : E \to F$ is *p-absolutely summing*, $0 < p < \infty$, if there exist an absolutely convex neighborhood U of 0 in E and a bounded quasi-absolutely convex subset B of F such that $S_0 : E_U \to F_B$ is p-absolutely summing. This definition is analogous with the definition of nuclear operators on locally convex spaces (see [27]).

The next result gives sufficient conditions for p-decomposability of cylindrical elements. It is an extension of the Kwapien's Theorem ([28], Th. 2) as well as ([25], Th. 1.1) on the case of absolutely summing operators on locally convex spaces. Moreover, the method of absolutely summing operators on locally convex spaces allows to simplify the proof of ([28], Th. 2) and contains the case $0 < p < 1$.

Theorem 3. Let E, F be a quasi-complete l.c.s. and let $S : E \to F$ be p-absolutely summing linear operator, $p > 0$. If $X : E'_\tau \to L^p$ is a continuous cylindrical element and either $p \geq 1$ or F' has the approximation property then

(i) $Y = X \circ S^*$ is p-decomposable by an F valued function $y(\cdot)$
(ii) If L^p is separable then for each absolutely convex neighborhood U of 0 in E and each continuous seminorm $\|\cdot\|$ on F we have

$$\int_\Omega \|y(\cdot)\|^p \, dP \leq C \int_{U^\circ} \|Xe'\|^p_{L^p} \, d\mu(e')$$

where μ is a Radon measure on $(U^\circ, \sigma(E', E))$ and C is some constant.

Proof. Let U be an absolutely convex closed neighborhood of 0 in E and B an absolutely convex closed subset of F such that $S_0 : E_U \to F_B$ is p-absolutely summing. Because F is quasi-complete, F_B is a Banach space and S_0 extends to the map $\bar{S}_0 : \hat{E}_U \to F_B$, which is also p-absolutely summing. Since $(E_U)' = (\hat{E}_U)' = E'_{U^\circ}$ and $(F_B)' = F'_{B^\circ}$, $(\bar{S}_0)^* = S_0^* : F'_{B^\circ} \to E'_{U^\circ}$. Moreover $\Psi_{V^\circ} : F'_{V^\circ} \to F'_\tau$ is continuous. Therefore applying Kwapien's Theorem ([28], Th.2) to the operators S_0^* and $X \circ \Psi_{V^\circ}$ acting on Banach spaces, we obtain that that $S_0^* X \Psi_{V^\circ}$ is p-decomposable by $y_B(\cdot) : \Omega \to (F'_B)' = F_B$ (if F' has the approximation property then also F'_{B° has it (cf. [27] III, 9.2). Using the continuity of the cannonical injection $\Psi_B : F_B \to F$ we see that the function

$$y(\cdot) = \Psi_B y_B(\cdot) : \Omega \to F$$

decomposes $X \circ S^*$. Furthermore, let us note that U° is the unit ball in the space $(E_U)'$ which is compact in $\sigma(E', E)$-topology. Thus using ([25] Th.1.1 (ii) we obtain the inequality

$$\int_\Omega \|y(\cdot)\|^p_B \, dP \leq C \int_{U^\circ} \|Xe'\|^p_{L^p} \, d\mu(e')$$

where the measure μ is defined as in Proposition 6. If $\|\cdot\|$ is a continuous seminorm on F then $\|\cdot\| \leq C_1 \|\cdot\|_{B'}$ for some constant C_1. This ends the proof of this theorem.

AUTHOR CONTRIBUTIONS

The author confirms being the sole contributor of this work and has approved it for publication.

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