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Scattering by singular potentials in coupled Schrödinger equations

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Scattering in pairs of one-dimensional time-independent Schrödinger equations coupled via singular potentials are considered. For potentials given by Dirac's delta function reflected and transmitted waves of the two modes as well as a bound state is found by integration. For potentials given by the derivative of Dirac's delta function resonant reflection and transmission occur for a discrete set of amplitudes of the scattering potential. These results depend on the applied regularization.

Keywords: one-dimensional two-mode quantum systems, singular potentials, resonant tunneling.

Dedicated to the memory of Yuri Gaididei

1. Introduction

In many textbooks on quantum mechanics, one finds the solution to the scattering problem for the one-dimensional time-independent Schrödinger equation with a potential given by Dirac's $\delta(x)$ function. Reflection and transmission coefficients for reflected and transmitted fields as well as the coefficient for the single-bound state are obtained by integration.

The corresponding problem for the derivative of the $\delta(x)$ function, $\delta'(x)$, cannot be solved by integration. Here Patil [1] demonstrated total reflection of the incident field by regularization of the δ' function. Using a different regularization of the potential Christiansen *et al*. [2] obtained resonant transmission for a discrete set of amplitudes of the singularity. Later Zolotaryuk *et al.* [3], Toyama and Nogami [4], and others demonstrated the nonuniqueness of the problem using generalized regularizations. Recently, Zolotaryuk and Zolotaryuk [5] even discovered the possibility of obtaining a bound state at the δ' potential by proper regularization. Additional references may be found in their work.

In paper [6], Zolotaryuk discusses the physical interpretation through single-point barriers based on a double-layer heterostructure in the squeezing limit as both the thickness of the layers and the distance between them tend to zero simultaneously. In this limit, the electron transmission through a barrier-well structure becomes non-zero for a discrete set of parameter values. However, it may be concluded that the Schrödinger equation with δ' potential only has a physical meaning when an additional specification of the regularization procedure is provided.

Here we shall consider pairs of one-dimensional time-independent Schrödinger equations that are coupled through singular potentials of the type: $\delta(x)$ and $\delta'(x)$. We solve the scattering problem for an incident field of one of the modes involved by integration in the δ case and by regularization in the δ' case. In the latter case the calculations are vastly simplified by introducing the stretched coordinate $\xi = x/\varepsilon$, where x is the space coordinate and ε a perturbation parameter. This technique for handling singular potentials was also applied in [7]. In the literature several studies of entanglement investigate coupled quantum systems, e.g., the linear coupling between a set of harmonic quantum oscillators giving rise to two coupled Schrödinger equations for the corresponding wave functions. (For references see Google: entanglement coupled Schrödinger equations [8].) The coupling may depend on the spatial variable, x. We present a case where the coupling is restricted to a single point $x = 0$, thus realized by a Dirac's delta function, $\delta(x)$, or by its derivative with respect to x, $\delta'(x)$.

The mathematical results are expected, after further specifications, also to find specific applications as models of electronic or optical devices involving double layers. Thus, one may have to resort to invoking the following general conclusion made by Dirac at a higher level in the Scientific American paper [9] in order to physically justify the mathematical research. Dirac writes: "It may well be that the next advance in physics will come about along these lines: people first discovering the equations and then needing a few years of development in order to find the physical ideas behind the equations".

2. Schrödinger equations with delta potentials

The one-dimensional time-independent Schrödinger equation with propagation constant k and the singular $\delta(x)$ well potential with strength $\rho > 0$

$$\frac{d^2\psi(x)}{dx^2} - \rho\delta(x)\psi(x) + k^2\psi(x) = 0 \tag{1}$$

can be solved by integration with respect to x leading to the conditions at $x = 0$

$$\psi(x)\,|_{0-}^{0+} = 0, \quad \psi'(x)\,|_{0-}^{0+} = \rho\psi(0). \tag{2}$$

For $x \neq 0$ (i.e., $\delta(x) \equiv 0$) we shall write the field $\psi(x)$ as the sum of an incident and a reflected field for $x < 0$ and a transmitted field for $x > 0$

$$\psi(x) = \begin{cases} \exp(ikx) + R\exp(-ikx), & x < 0, \\ T\exp(ikx), & x > 0, \end{cases} \tag{3}$$

where

$$R = -\frac{-i\rho/2}{k + i\rho/2}, \; T = \frac{k}{k + i\rho/2}, \tag{4}$$

satisfying Eqs. (2). It is noted that the energy is conserved since $|R|^2 + |T|^2 = 1$.

For $k = -i\rho/2$ there exists a bound state

$$\psi(x) = \begin{cases} A\exp\left(\frac{\rho x}{2}\right), & x < 0, \\ A\exp\left(-\frac{\rho x}{2}\right), & x > 0. \end{cases} \tag{5}$$

Since $\int_{-\infty}^{\infty} |\psi(x)|^2\, dx = 1$ one finds the coefficient $A = \sqrt{\rho/2}$.

These results are obtained in many text books on quantum mechanics. In addition it may be observed that A^2 = Residue $(1+R)_{k=-i\rho/2}$.

2.1. Coupled Schrödinger equations

We now consider a pair of Schrödinger equations for the waves $\psi_a(x)$ and $\psi_b(x)$, with identical propagation constant k, which are coupled via the singular potential $-\rho\delta(x)$ with $\rho > 0$

$$\frac{d^2\psi_a(x)}{dx^2} - \rho\delta(x)\psi_b(x) + k^2\psi_a(x) = 0, \tag{6a}$$

$$\frac{d^2\psi_b(x)}{dx^2} - \rho\delta(x)\psi_a(x) + k^2\psi_b(x) = 0, \tag{6b}$$

$$-\infty < x < \infty$$

with Lagrangian

$$L = \left(\frac{d\psi_a(x)}{dx}\right)^2 + \left(\frac{d\psi_b(x)}{dx}\right)^2 - \frac{k^2}{2}\psi_a(x)^2$$

$$-\frac{k^2}{2}\psi_b(x)^2 + \rho\delta(x)\psi_a(x)\psi_b(x). \tag{7}$$

Proceeding as in the previous case we get by integration of Eqs. (6)

$$\psi_a(x)\,|_{0-}^{0+} = 0, \quad \psi_a'(x)\,|_{0-}^{0+} = \rho\psi_b(0),$$

$$\psi_b(x)\,|_{0-}^{0+} = 0, \quad \psi_b'(x)\,|_{0-}^{0+} = \rho\psi_a(0). \tag{8}$$

Writing $\psi_a(x)$ as the sum of an incoming and a reflected field and a transmitted field, and $\psi_b(x)$ as a reflected and a transmitted field

$$\psi_a(x) = \begin{cases} \exp(ikx) + R_a\exp(-ikx), & x < 0, \\ T_a\exp(ikx), & x > 0, \end{cases} \tag{9a}$$

$$\psi_b(x) = \begin{cases} R_b\exp(-ikx), & x < 0, \\ T_b\exp(ikx), & x > 0, \end{cases} \tag{9b}$$

we find

$$R_a = \frac{-\rho^2}{4k^2 + \rho^2}, \; T_a = \frac{4k^2}{4k^2 + \rho^2}, \; R_b = T_b = \frac{-2ik\rho}{4k^2 + \rho^2}, \tag{10}$$

satisfying Eqs. (8). Again, the energy is conserved since $|R_a|^2 + |T_a|^2 + |R_b|^2 + |T_b|^2 = 1$.

For $k = \pm i\rho/2$ there exist bound states

$$\psi_a(x) = \begin{cases} A\exp\left(\frac{\rho x}{2}\right), & x < 0, \\ A\exp\left(-\frac{\rho x}{2}\right), & x > 0, \end{cases} \quad (11a)$$

$$\psi_b(x) = \begin{cases} B\exp\left(\frac{\rho x}{2}\right), & x < 0, \\ B\exp\left(-\frac{\rho x}{2}\right), & x > 0. \end{cases} \quad (11b)$$

Since $\int_{-\infty}^{\infty} (|\psi_a(x)|^2 + |\psi_b(x)|^2)dx = 1$ one finds the coefficients $A = \sqrt{\rho}/2$ and $B = \sqrt{\rho}/2$.

Here $A^2 =$ Residue $(1+R_a)_{k=\pm i\rho/2} = \rho/4$ and $B^2 =$ = Residue $(R_b)_{k=\pm i\rho/2} = \rho/4$.

3. Schrödinger equations with delta prime potentials

Replacing the singular potential in Eq. (1) $-\rho\delta(x)$ by $\tau^2\delta'(x)$ we obtain

$$\frac{d^2\psi(x)}{dx^2} + \tau^2\delta'(x)\psi(x) + k^2\psi(x) = 0. \quad (12)$$

Integration with respect to x immediately leads to contradiction as shown in Refs. 1 and 2. Instead we regularize the problem, as in Ref. 2, replacing $\delta'(x)$ by $\Delta'(x)$ given by

$$\Delta'(x) = \begin{cases} 1/\varepsilon^2, & -\varepsilon < x < 0 \\ -1/\varepsilon^2, & 0 < x < \varepsilon \\ 0, & |x| > \varepsilon \end{cases} \quad (13)$$

in the limit $\varepsilon \to 0$. For $x \neq 0$ we write the field $\psi(x)$ as the sum of an incident and a reflected field for $x < 0$ and a transmitted field for $x > 0$ as in Eq. (3), and it was found

$$R = -1, \quad T = 0, \text{ for } \tan\tau \neq \tanh\tau, \quad (14a)$$

$$R = \tan^2\tau, \quad T = 1/(\cos\tau\cosh\tau), \text{ for } \tan\tau = \tanh\tau. \quad (14b)$$

Thus resonant transmission occurs for the discrete set of τ-values satisfying the condition

$$\tan\tau = \tanh\tau. \quad (15)$$

Note: $|R|^2 + |T|^2 = 1$.

3.1. Coupled Schrödinger equations

Replacing the singular potential $-\rho\delta(x)$ by $\tau^2\delta'(x)$ in Eqs. (6) the resulting pair of equations

$$\frac{d^2\psi_a(x)}{dx^2} + \tau^2\delta'(x)\psi_b(x) + k^2\psi_a(x) = 0, \quad (16a)$$

$$\frac{d^2\psi_b(x)}{dx^2} + \tau^2\delta'(x)\psi_a(x) + k^2\psi_b(x) = 0, \quad (16b)$$

$$-\infty < x < \infty$$

with Lagrangian

$$L = \left(\frac{d\psi_a(x)}{dx}\right)^2 + \left(\frac{d\psi_b(x)}{dx}\right)^2 - \frac{k^2}{2}\psi_a(x)^2 - \frac{k^2}{2}\psi_b(x)^2 - \tau^2\delta'(x)\psi_a(x)\psi_b(x), \quad (17)$$

leads to contradiction when integrated. Again we regularize by replacing $\delta'(x)$ by $\Delta'(x)$ given by Eq. (13) and write $\psi_a(x)$ as the sum of an incoming and a reflected field and a transmitted field, and $\psi_b(x)$ as a reflected and a transmitted field

$$\psi_a(x) = \begin{cases} \exp(ikx) + R_a\exp(-ikx), & x < -\varepsilon, \\ T_a\exp(ikx), & x > \varepsilon, \end{cases} \quad (18a)$$

$$\psi_b(x) = \begin{cases} R_b\exp(-ikx), & x < -\varepsilon, \\ T_b\exp(ikx), & x > \varepsilon. \end{cases} \quad (18b)$$

Introducing the stretched variable $\xi = x/\varepsilon$ as in [7] in the interval $-\varepsilon < x < \varepsilon$ we may write Eqs. (16) with Eq. (13) as

$$\frac{d^2\psi_a(\xi)}{d\xi^2} + \tau^2\psi_b(\xi) = 0, \quad \frac{d^2\psi_b(\xi)}{d\xi^2} + \tau^2\psi_a(\xi) = 0,$$

$$-1 < \xi < 0, \quad (19a)$$

$$\frac{d^2\psi_a(\xi)}{d\xi^2} - \tau^2\psi_b(\xi) = 0, \quad \frac{d^2\psi_b(\xi)}{d\xi^2} - \tau^2\psi_a(\xi) = 0,$$

$$0 < \xi < 1 \quad (19b)$$

in the limit $\varepsilon \to 0$.

Noting

$$\frac{d^4\psi_a(x)}{d\xi^4} - \tau^4\psi_a(\xi) = 0 \quad (20)$$

as well as Eqs. (16) we may write the solutions to Eqs. (19), $\psi_a(x)$ with upper sign and $\psi_b(x)$ with the lower sign:

$$\psi_{\substack{a\\b}}(\xi) = (A_{-,0} + \varepsilon A_{-,1} + \varepsilon^2 A_{-,2})\sin\tau(\xi+1) + (B_{-,0} + \varepsilon B_{-,1} + \varepsilon^2 B_{-,2})\cos\tau(\xi+1)$$

$$\pm (C_{-,0} + \varepsilon C_{-,1} + \varepsilon^2 C_{-,2})\sinh\tau(\xi+1) \pm (D_{-,0} + \varepsilon D_{-,1} + \varepsilon^2 D_{-,2})\cosh\tau(\xi+1), \quad -1 < \xi < 0, \quad (21a)$$

$$\psi_{\substack{a\\b}}(\xi) = \pm(A_{+,0} + \varepsilon A_{+,1} + \varepsilon^2 A_{+,2})\sin\tau(\xi-1) \pm (B_{+,0} + \varepsilon B_{+,1} + \varepsilon^2 B_{+,2})\cos\tau(\xi-1)$$

$$+ (C_{+,0} + \varepsilon C_{+,1} + \varepsilon^2 C_{+,2})\sinh\tau(\xi-1) + (D_{+,0} + \varepsilon D_{+,1} + \varepsilon^2 D_{-,2})\cosh\tau(\xi-1), \quad 0 < \xi < 1, \quad (21b)$$

where the coefficients A_-, B_-, C_-, and D_- $(-1<\xi<0)$ and A_+, B_+, C_+, and D_+ $(0<\xi<1)$ are expanded from zeroth to second order in ε. Thus, there are 24 of these expansion coefficients.

Satisfying continuity conditions for $\psi_a(x)$, $d\psi_a(x)/dx$, $\psi_b(x)$, and $d\psi_b(x)/dx$ at $x=-\varepsilon$ (alias $\xi=-1$) and $x=\varepsilon$ (alias $\xi=1$) to orders ε^0, ε^1, and ε^2 facilitates elimination of the 24 expansion coefficients using *Mathematica*. Here it should be noted that $d\psi_a(\xi)/dx$ and $d\psi_b(\xi)/dx$ becomes of order ε^{-1} at $\xi=-1$ and $\xi=1$. In order to avoid such singularities as $\varepsilon\to 0$ $A_{-,0}=0$, $C_{-,0}=0$, $A_{+,0}=0$, and $C_{+,0}=0$ must be required.

Satisfying also continuity conditions for $\psi_a(x)$, $d\psi_a(x)/dx$, $\psi_b(x)$, and $d\psi_b(x)/dx$ at $x=0$ (alias $\xi=0$) to orders ε^0, ε^1, and ε^2 we get the 12 equations for R_a, R_b, T_a, and T_b to orders ε^0, ε^1, and ε^2

$$\mathbf{M}\cdot\begin{pmatrix}R_a\\R_b\\T_a\\T_b\end{pmatrix}=\mathbf{N}, \tag{22}$$

where $\mathbf{M}$ denotes a 4×4 matrix, and $\mathbf{N}$ is a 4×4 column vector. All elements of $\mathbf{M}$ and $\mathbf{N}$ are determined to orders ε^0, ε^1, and ε^2.

Solving Eq. (22) by Cramer's rule by means of *Mathematica* gives

$$R_a=N_{R_a}/M,\ R_b=N_{R_b}/M,$$

$$T_a=N_{T_a}/M,\ \text{and}\ T_b=N_{T_b}/M, \tag{23}$$

where

$$\begin{aligned}M\equiv|\mathbf{M}|=&\\ &-\tau^2(\cosh\tau\sin\tau-\cos\tau\sinh\tau)^2\ \varepsilon^0\\ &-4ik\tau(\cosh\tau\sin\tau-\cos\tau\sinh\tau)(\cosh\tau(\cos\tau+\tau\sin\tau)-\tau\cos\tau\sinh\tau)\ \varepsilon^1\\ &+2k^2(\cosh^2\tau(2\cos^2\tau+8\tau\cos\tau\sin\tau+(-1+4\tau^2\sin^2\tau)+\cos\tau((1+4\tau^2)\cos\tau\sinh^2\tau\\ &-4\tau(\cos\tau+\tau\sin\tau)\sinh 2\tau)))\ \varepsilon^2,\end{aligned} \tag{24}$$

$$\begin{aligned}N_{R_a}=&\\ &\tau^2(\cosh\tau\sin\tau-\cos\tau\sinh\tau)\ \varepsilon^0\\ &+2ik\tau(\cosh\tau\sin\tau-\cos\tau\sinh\tau)(\cosh\tau\,(\cos\tau+\tau\sin\tau)-\tau\cos\tau\sinh\tau)\ \varepsilon^1\\ &-\frac{k^2}{8}((\cosh\tau\sin\tau-\cos\tau\sinh\tau)\\ &+(2+\cos 2\tau+\cosh^2\tau+\tau\cos\tau\sin\tau-15\tau\cos\tau\sinh\tau+\sinh^2\tau\\ &+\cosh\tau(28\cos\tau+15\tau\sin\tau-\tau\sinh\tau)))\ \varepsilon^2,\end{aligned} \tag{25}$$

$$\begin{aligned}N_{R_b}=&\\ &0\ \varepsilon^0\\ &-2ik\tau\sin\tau\sinh\tau(\cosh\tau\sin\tau-\cos\tau\sinh\tau)\ \varepsilon^1\\ &+\frac{1}{8}k^2(-\tau\,(\cos\tau+\cosh\tau)(2\cos\tau-2\cosh\tau+\tau\sin\tau+\tau\sinh\tau)(-\cosh\tau\sin\tau+\cos\tau\sinh\tau)\\ &+32\sin\tau\sinh\tau(\cosh\tau(\cos\tau+\tau\sin\tau)-\tau\cos\tau\sinh\tau))\ \varepsilon^2,\end{aligned} \tag{26}$$

$$\begin{aligned}N_{T_a}=&\\ &0\ \varepsilon^0\\ &-2ik\tau\,(\cosh\tau\sin\tau-\cos\tau\sinh\tau)\ \varepsilon^1\\ &+\frac{1}{8}k^2(32\cosh\tau(\cos\tau+\tau\sin\tau)-32\tau\cos\tau\sinh\tau-\tau\,(\cos\tau-\cosh\tau)\\ &+(2\cos\tau-2\cosh\tau+\tau\sin\tau+\tau\sinh\tau)(-\cosh\tau\sin\tau+\cos\tau\sinh\tau))\ \varepsilon^2,\end{aligned} \tag{27}$$

and

$$N_{T_b} =$$
$$0\,\varepsilon^0$$
$$+\,0\,\varepsilon^1$$
$$-\frac{1}{8}k^2\tau\,((\cos\tau+\cosh\tau)(2\cos\tau-2\cosh\tau+\tau\sin\tau+\tau\sinh\tau)$$
$$+(-\cosh\tau\sin\tau+\cos\tau\sinh\tau))\,\varepsilon^2. \quad (28)$$

In the limit $\varepsilon \to 0$ and $\tan\tau \neq \tanh\tau$ we find from Eqs. (23) and (24)–(28)

$$R_a = -1,\ R_b = 0,\ T_a = 0,\ T_b = 0, \quad (29)$$

i.e., total reflection of the incident ψ_a mode into the reflected ψ_a mode.

In the same limit we obtain for $\tan\tau = \tanh\tau$

$$R_a = 0,\ R_b = \tan^2\tau,$$
$$T_a = 1/(\cosh\tau\cos\tau),\ T_b = 0. \quad (30)$$

Thus resonant transmission again occurs for the discrete set of τ-values satisfying the same transcendental equation (15) as in the single mode case. However, the incident ψ_a field is partly converted into a reflected ψ_b field, partly transmitted as a ψ_a field. There is thus no reflection into the ψ_a mode and no transmission into to ψ_b mode.

The energy is conserved since

$$|R_a|^2 + |T_a|^2 + |R_b|^2 + |T_b|^2 = 1.$$

4. Conclusions

We have solved the scattering problem for pairs of Schrödinger equations coupled via the singular δ and δ' potentials. In the former case reflected and transmitted fields, as well as a bound state, are uniquely determined by integration. In the latter case, integration is not possible. Non-unique results are obtained by a rectangular regularization of the $\delta'(x)$ potential.

We find the total reflection of the incident mode except for a discrete set of amplitudes for the δ' potential, where one part of the incident ψ_a field is converted into a reflected ψ_b field, and the other part is transmitted as a ψ_a field. Reflection and transmission coefficients are of similar form as in the single mode case.

The determination of these coefficients by perturbation theory requires the solution of 36 equations with 36 unknowns with an application of a stretched coordinate in the potential regularization.

The method is similar to the one applied in the beam problem considered in Ref. 10, where a fourth-order wave equation with a $\delta'''(x)$ singularity was solved using *Mathematica*. This could only be done numerically. In the present case, *Mathematica* provides analytical expressions.

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Розсіяння на сингулярних потенціалах у зв'язаних рівняннях Шредінгера

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Розглядається розсіяння в парах одновимірних незалежних від часу рівнянь Шредінгера, пов'язаних через сингулярні потенціали. Для потенціалів, заданих дельта-функцією Дірака, відбиті та ті, що пройшли, хвилі двох мод, а також зв'язаний стан знайдено шляхом інтегрування. Для потенціалів, заданих похідною дельта-функції Дірака, резонансне відображення та пропускання відбуваються для дискретного набору амплітуд потенціалу розсіяння. Ці результати залежать від застосованої регуляризації.

Ключові слова: одновимірні двомодові квантові системи, сингулярні потенціали, резонансне тунелювання.