On Scattering from the One Dimensional Multiple Dirac Delta Potentials

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Abstract

In this paper, we propose a pedagogical presentation of the Lippmann-Schwinger equation as a powerful tool so as to obtain important scattering information. In particular, we consider a one dimensional system with a Schrödinger type free Hamiltonian decorated with a sequence of N attractive Dirac delta interactions. We first write the Lippmann-Schwinger equation for the system and then solve it explicitly in terms of an $N \times N$ matrix. Then, we discuss the reflection and the transmission coefficients for arbitrary number of centers and study threshold anomaly for $N = 2$ and $N = 4$ cases. We also study further features like quantum metastable states like resonances, including their corresponding Gamow functions, and virtual or antibound states. The use of the Lippmann-Schwinger equation simplifies enormously our analysis and gives exact results for an arbitrary number of Dirac delta potential.

1 Introduction

As a special case of point interactions, Dirac delta potential has been taking interest for many years. A well-known application of delta potentials in physics is the Dirac comb in the Kronig Penney model which explains band gap formation in crystal structures [1]. Another important application of delta potential is the description of the interaction between weakly interacting bosons through the Dirac delta functions (see e.g. Chapter 15 in [2] and references therein). The successful physical applications of delta potentials lead to a considerable amount of work about Dirac delta potentials in the different areas of physics (see [3, 4] and references therein). A remarkable study among them shows that scattering and reflection amplitudes of an arbitrary potential can be approximated using delta potentials [5]. More recently, studies of one-dimensional several Dirac delta potentials based on transfer matrix techniques have been developed to illustrate some interesting scattering phenomenon, namely the so-called transmission resonances (the energies for which the scattering transmission coefficient is one), threshold anomalies (for the particular values of the parameters, the reflection coefficient goes to zero as the energy of the incoming particle approaches zero), Bloch states [6, 7, 8, 9, 10, 11], etc.

Another important point about Dirac delta potentials is that they are exactly solvable. This makes them also useful for teaching purposes. Green's functions and the solution of the Lippmann-Schwinger equation for a single Dirac delta potential has been given in [12] and multiple scattering theory for double delta centers has been studied through the Lippmann-Schwinger equation in [13], from a pedagogical point of view. A recent review [3] has illustrated some other interesting features of the one-dimensional Dirac delta potentials, in particular the continuum and the bound state spectrum of delta potentials together with some other exactly solvable potentials. In there, multiple δ-function potential has been studied in Fourier space and the bound state problem has been formulated in terms of a matrix eigenvalue problem.

In this paper, we study the details of the scattering spectrum of the multiple Dirac delta potentials through the solution of the Lippmann-Schwinger equations, which make use of Green functions. We give here another point of view for the treatment of the model introduced in [6, 10]. Our point of departure is the Lippmann-Schwinger equation and we shall show how to calculate the scattering coefficients for a system of N Dirac delta potentials. The method is based on the exact solution of the Lippmann-Schwinger equations rather than solving system of equations using the boundary conditions for delta potentials at each delta center [10]. The method that utilizes the boundary conditions becomes rather cumbersome for $N > 2$, whereas the method used here is more systematic and the results can easily be obtained for an arbitrary number of centers. Therefore, our results also suggest the use of Lippmann-Schwinger equation for classroom exercises including one dimensional solvable models (e.g., multiple Dirac delta potentials), which are crucial when teaching quantum scattering.

The threshold anomaly is defined as a nonzero probability of transmission through a potential barrier as the kinetic energy of the incident particles approaches to zero [7]. Therefore its existence is investigated by analysing the behavior of the reflection $R(k)$ or transmission probabilities $T(k)$ for small values of k. It is shown in [7] that this phenomena is related to the formation of new bound states for the given potential barrier. In this paper, we explicitly illustrate this phenomena for two and four centers.

Contact potentials and particularly those given by two or more Dirac deltas serve also to model quantum systems with resonances defined as quantum unstable states or/and virtual states (also called anti-bound states) [14, 15, 16, 17, 18, 19]. The resonances can be determined from the position of the poles of S-matrix in complex energy or momentum plane. In this manuscript, instead of paying attention to find the values of resonance poles, we focus on obtaining the Gamow functions (vectors) or eigenfunctions (eigenvectors) for the exponentially decaying part of a resonance as a direct conclusion of the Lipmann-Schwinger equation in a straightforward way. These Gamow vectors are interesting, for instance, in order to construct spectral expansion for the total Hamiltonian producing quantum decaying states. We also show the appearance of the virtual states for $N = 2$.

The paper is organized as follows: In Section 2, starting with the Lippmann-Schwinger equation as a point of departure, we provide the solution of it in terms of an $N \times N$ matrix. The scattering information (transmission and reflection probabilities) are discussed in Section 3 with particular emphasis on the simple models with one or two Dirac deltas. In Section 4, we discuss the threshold anomaly for two and four Dirac delta centers. In Section 5, we recall the basic definitions and features of resonances as quantum unstable states. From the Lippmann-Schiwinger equation, we readily obtain the Gamow functions explicitly in this case. Finally, we discuss the appearance of the virtual (anti-bound) states for two centers. We also summarize the bound state formalism of the problem in Appendix A.

2 The Lipmann-Schwinger equation for N Dirac delta potentials

Let us start 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 potential V, so that the total Hamiltonian is $H = H_0 + V$. In our analysis, we consider the Lippmann-Schwinger equation in momentum space. This has the advantage of its simplicity, which helps very much in practical calculations as well as in its conceptual clarity. This equation can be written in the following form [20]

$$|k^\pm\rangle = |k\rangle - G_0(E_k \pm i0)V|k^\pm\rangle \,, \tag{1}$$

where $E_k = k^2/2m$. The operator $G_0(z) = (H_0 - z)^{-1}$ is called the Green operator for H_0 and has interesting properties. First of all, it is an analytic function on the complex variable z, except at the values of the continuous spectrum of H_0, i.e., the positive semiaxis $\mathbb{R}^+ \equiv [0, \infty)$. This means that for any vectors φ, ψ in the Hilbert space $\mathcal{H}$, in which H_0 and H act, the functions $g_{\varphi,\psi}(z)$ given by the scalar products $g_{\varphi,\psi}(z) = \langle\varphi|(H_0 - z)^{-1}\psi\rangle$ are analytic on the mentioned domain that we denote as $\mathbb{C}/\mathbb{R}^+$. Then, $G_0(E_k \pm i0)$ are the boundary values of $G_0(z)$ on the positive real line when we approach from above (plus sign) or from below (minus sign). This idea is more often expressed as, $\lim_{\epsilon\to 0^+} G_0(E_k \pm i\epsilon) = G_0(E_k \pm i0)$. Since the Green's operator is discontinuous for the values of the spectrum of the free Hamiltonian, the positive semiaxis in our case, both limits are different [20].

We tacitly assume that the *continuous* spectrum of H is also $\mathbb{R}^+$. Concerning the kets $|k\rangle$ and $|k^\pm\rangle$, they are eigenvectors of H_0 and H, respectively, i.e., $H_0|k\rangle = k|k\rangle$ and $H|k^\pm\rangle = k|k^\pm\rangle$ for k in the continuous spectrum of both operators. The signs $\pm$ correspond to incoming $-$ and outgoing $+$ wave functions. It is well known that these state vectors are represented by plane waves which are not normalizable in the Hilbert space sense. Therefore, they do not belong to $\mathcal{H}$, but instead are defined as elements of a bigger structure that encompass $\mathcal{H}$, the so-called rigged Hilbert space [21, 22, 23, 24, 25, 26, 27].

We first write the potential V in the bra-ket formalism. If $|x\rangle$ are the position eigen-kets with real eigenvalue x and ψ is any state vector, we know that the wave function $\psi(x)$ for ψ can be written as $\psi(x) = \langle x|\psi\rangle$. Now, for simplicity, let us assume that $V(x) = \lambda\delta(x - a)$. The action of V on the wave function $\psi(x)$ is

$$(V\psi)(x) = \lambda\delta(x - a)\psi(x) = \lambda\delta(x - a)\psi(a) \,. \tag{2}$$

Note that $(V\psi)(x) = \langle x|V\psi\rangle$ and that for a fixed and all x, $\langle x|a\rangle = \delta(x-a)$. Then, if $V = \lambda|a\rangle\langle a|$, we may write

$$\langle x|V\psi\rangle = \lambda\langle x|a\rangle\langle a|\psi\rangle = \lambda\delta(x-a)\psi(a)\,. \tag{3}$$

Hence, we conclude that the operator "multiplication times the Dirac delta $\delta(x-a)$" can be written in the bra-ket language as $|a\rangle\langle a|$.

This can be generalized to N Dirac delta potentials located at different points a_i with different strengths λ_i, namely

$$V = -\sum_{i=1}^{N} \lambda_i |a_i\rangle\langle a_i|\,. \tag{4}$$

If we insert equation (4) into equation (1) and multiply the result from the left by the bra $\langle x|$, we obtain:

$$\langle x|k^{\pm}\rangle = \langle x|k\rangle + \sum_{j=1}^{N} \lambda_i \langle x|G_0(E_k \pm i0)|a_j\rangle\langle a_j|k^{\pm}\rangle\,. \tag{5}$$

Recall that $\langle x|k\rangle$ is the free plane wave and we keep only the sign $+$ in equation (5). Then, we find the following equation for the perturbed plane wave $\psi_k^+(x) = \langle x|k^+\rangle$ as

$$\psi_k^+(x) = e^{ikx} + \sum_{j=1}^{N} \lambda_j\, G_0(x, a_j; E_k + i0)\, \psi_k^+(a_j)\,, \tag{6}$$

where we have used the notation $G_0(x, y; E_k + i0) = \langle x|G_0(E_k + i0)|y\rangle$. This is the well known Green's function for the free Hamiltonian H_0 [20].

In order to have the explicit form for $\psi_k^+(x)$, we need to find $\psi_k^+(a_j)$. To do it, we just replace x by a_i in equation (6) and isolate the $j = i$ th term from the sum:

$$\psi_k^+(a_i) = e^{ika_i} + \lambda_i\, G_0(a_i, a_i; E_k + i0)\, \psi_k^+(a_i) + \sum_{j\neq i}^{N} \lambda_j\, G_0(a_i, a_j; E_k + i0)\, \psi_k^+(a_j)\,, \tag{7}$$

or

$$\psi_k^+(a_i)[1 - \lambda_i\, G_0(a_i, a_i : E_k + i0)] - \sum_{j\neq i}^{N} \lambda_j\, G_0(a_i, a_j; E_k + i0)\psi_k^+(a_j) = e^{ika_i}\,. \tag{8}$$

This relation can be written in a matrix form.

$$\sum_{j=1}^{N} \Phi_{ij}(E_k + i0)\, \psi_k^+(a_j) = e^{ika_i}\,, \qquad i = 1, 2, \dots, N\,, \tag{9}$$

where the Φ_{ij}'s are the matrix elements of the matrix $\Phi = \{\Phi_{ij}\}$, given by

$$\Phi_{ij}(E_k + i0) = \begin{cases} 1 - \lambda_i\, G_0(a_i, a_i : E_k + i0) & \text{if} \quad i = j\,, \\ -\lambda_j\, G_0(a_i, a_j; E_k + i0) & \text{if} \quad i \neq j\,. \end{cases} \tag{10}$$

The solution of equation (9) can be easily obtained as

$$\psi_k^+(a_j) = \sum_{j=1}^{N} [\Phi^{-1}(E_k + i0)]_{ji}\, e^{ika_i}\,, \tag{11}$$

where Φ^{-1} is the inverse of the matrix Φ. If we substitute equation (10) in equation (6), we find

$$\psi_k^+(x) = e^{ikx} + \sum_{i,j=1}^{N} \lambda_i\, G_0(x, a_i; E_k + i0)\, [\Phi^{-1}(E_k + i0)]_{ij}\, e^{ika_j}$$

$$. \tag{12}$$

To calculate $\psi_k^+(x)$ explicitly, we first find the free Green's function $G_0(x, a_i; E_k + i0)$. We insert a complete set of eigenkets of the momentum operator, $I = \int_{-\infty}^{\infty} |p\rangle\langle p|\, dp/2\pi\hbar$:

$$G_0(x, a_i; E_k + i0) = \langle x|G_0(E_k + i0)|a_i\rangle = \int_{-\infty}^{\infty} \langle x|G_0(E_k + i0)|p\rangle\langle p|a_i\rangle \, \frac{dp}{2\pi\hbar} \,. \tag{13}$$

By definition, $|p\rangle$ are the eigenkets of the momentum operator, so that $H_0|p\rangle = \frac{p^2}{2m}|p\rangle$. Then,

$$\langle x|G_0(E_k + i0)|p\rangle = \langle x|(H_0 - (E_k + i0))^{-1}|p\rangle = \langle x|\frac{1}{\frac{p^2}{2m} - (E_k + i0)}|p\rangle = \frac{1}{\frac{p^2}{2m} - (E_k + i0)} \, e^{ipx/\hbar} \,. \tag{14}$$

Using $\langle p|a_i\rangle = e^{-ipa_i/\hbar}$ and equation (14) in equation (13), we have the following expression for (13):

$$\int_{-\infty}^{\infty} \frac{e^{ip(x-a_i)/\hbar}}{\frac{p^2}{2m} - (E_k + i0)} \, \frac{dp}{2\pi\hbar} = \frac{m}{\pi\hbar} \int_{-\infty}^{\infty} \frac{e^{ip(x-a_i)/\hbar}}{p^2 - 2m(E_k + i0)} \, dp \,. \tag{15}$$

Before we proceed to the next step, let us recall that

$$G_0(x, a_i; E_k + i0) = \lim_{\epsilon \to 0^+} G_0(x, a_i; E_k + i\epsilon) \,. \tag{16}$$

This remark is essential in order to understand the meaning of the integral in (15), which is nothing else that:

$$\int_{-\infty}^{\infty} \frac{e^{ip(x-a_i)/\hbar}}{p^2 - 2m(E_k + i0)} \, dp = \lim_{\epsilon \to 0^+} \int_{-\infty}^{\infty} \frac{e^{ip(x-a_i)}}{p^2 - 2m(E_k + i\epsilon)} \, dp \,. \tag{17}$$

It is very important to understand that the limit and the integral in (17) cannot be interchanged since it is the right hand side of (17) that gives sense to the left hand side. In fact, we have to solve the integral first and then proceed with the limit. Let us solve the integral in the right hand side of (17) by the residue method. The function under the integral sign has poles at the points

$$p = \pm\hbar k \sqrt{1 + i \, \frac{2m\epsilon}{\hbar^2 k^2}} \simeq \pm \left(\hbar k + i \, \frac{m\epsilon}{\hbar k}\right) \,, \tag{18}$$

where $E_k = \hbar^2 k^2/2m$ and $k > 0$. In order to calculate the integral by the residue method, we have to take into account that either $x < a_i$ or $x > a_i$. In the second case, we use the contour depicted in the left contour of Figure 1. We note that only the pole with plus sign in equation (18) lies inside the contour of integration. The

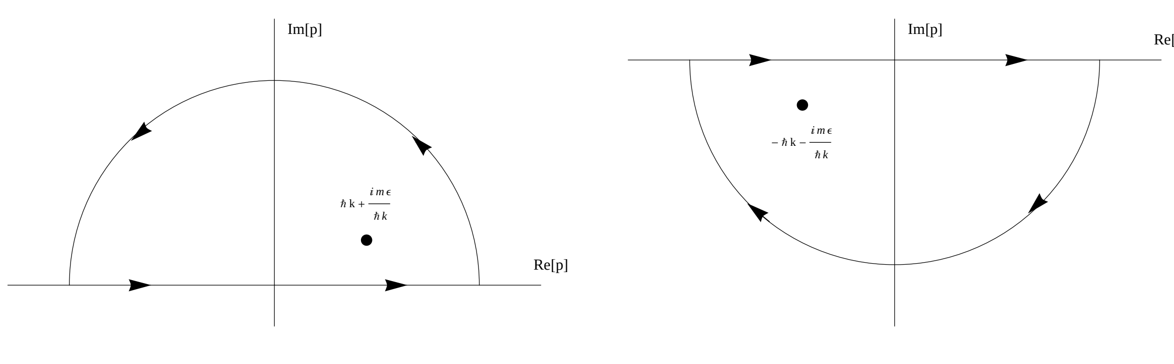

Figure 1: We choose the left contour for the residue calculation for $x > a_i$, and the right one for $x < a_i$.

integral over the semicircle vanishes as its radius goes to infinite [28]. Then, the value of the integral is obtained multiplying by $2\pi i$ the residue at that point. This gives:

$$i\frac{m}{\hbar} \left[\lim_{\epsilon \to 0^+} \frac{e^{i(k + \frac{m\epsilon}{k})(x-a_i)}}{\hbar k + i \, \frac{m\epsilon}{\hbar k}} \right] = im \, \frac{e^{ik(x-a_i)}}{\hbar^2 k} \,. \tag{19}$$

This is the result of the integral (17) for $x > a_i$. For $x < a_i$ we use a similar contour defined in the lower half plane, as shown in the right contour of Figure 1. Then, the relevant pole is the one with minus sign in equation

(18). This gives a similar result as in (19), replacing the k in the exponential by $-k$. Therefore, for all values of x we can write:

$$G_0(x, a_i; E_k + i0) = \int_{-\infty}^{\infty} \frac{e^{ip(x-a_i)/\hbar}}{\frac{p^2}{2m} - (E_k + i0)} \frac{dp}{2\pi\hbar} = \frac{im}{\hbar^2 k} e^{k|x-a_i|} . \tag{20}$$

Substituting this result into the formula (12), we finally obtain

$$\psi_k^+(x) = e^{ikx} + \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{im\sqrt{\lambda_i \lambda_j}}{\hbar^2 k} e^{ik|x-a_i|} [\Phi^{-1}(E_k + i0)]_{ij} e^{ika_j} , \tag{21}$$

where

$$\Phi_{ij}(E_k + i0) = \begin{cases} 1 - \frac{im\lambda_i}{\hbar^2 k} & \text{if} \quad i = j , \\ -\sqrt{\lambda_i \lambda_j} \frac{im}{\hbar^2 k} e^{ik|a_i - a_j|} & \text{if} \quad i \neq j . \end{cases} \tag{22}$$

Note that $\Phi^{-1}(E + i0)$ is the inverse of the matrix with elements given above equation (22).

3 The Reflection and the Transmission Coefficients

We assume that the incoming particles come from left. Then, from the coefficient of e^{-ikx} in the solution $\psi_k^+(x)$ when $x < a_i$, we can find the reflection amplitude

$$r(k) = \sum_{i,j=1}^{N} \frac{im\sqrt{\lambda_i \lambda_j}}{\hbar^2 k} e^{ika_i} [\Phi^{-1}(E_k + i0)]_{ij} e^{ika_j} , \tag{23}$$

and from the coefficient of e^{ikx} in the solution $\psi_k^+(x)$ for $x > a_i$, we can find the transmission amplitude

$$t(k) = 1 + \sum_{i,j=1}^{N} \frac{im\sqrt{\lambda_i \lambda_j}}{\hbar^2 k} e^{-ika_i} [\Phi^{-1}(E_k + i0)]_{ij} e^{ika_j} . \tag{24}$$

It is instructive to show that the solution $\psi_k^+(x)$, and the reflection and the transmission amplitudes given above yield to the standard textbook results if we consider one Dirac delta potential located at $x = a$ with strength λ.

For $N = 1$, the matrix Φ is simply a function, namely

$$\Phi_{11}(E_k + i0) = 1 - \frac{im\lambda}{\hbar^2 k} , \tag{25}$$

where we have chosen $\lambda_1 = \lambda$ and used $\lim_{\epsilon \to 0^+} \sqrt{-2m(E_k + i\epsilon)} = -i\hbar k$. Then, the above formula (21) is reduced to

$$\psi_k^+(x) = \begin{cases} e^{ikx} + \frac{im\lambda}{\hbar^2 k} \frac{e^{-ik(x-a)}}{1 - i\frac{m\lambda}{\hbar^2 k}} & \text{if } x < a , \\ \\ e^{ikx} + \frac{im\lambda}{\hbar^2 k} \frac{e^{ik(x-a)}}{1 - i\frac{m\lambda}{\hbar^2 k}} & \text{if } x > a . \end{cases} \tag{26}$$

Substituting the function Φ given in Eq.(25) into Eqs. (23) and (24), we obtain the following well-known textbook result [29]:

$$R(k) = |r(k)|^2 = \frac{m^2 \lambda^2}{\hbar^4 k^2 + m^2 \lambda^2} , \qquad T(k) = |t(k)|^2 = \frac{\hbar^4 k^2}{\hbar^4 k^2 + m^2 \lambda^2} . \tag{27}$$

Note that $R + T = 1$. Moreover, $T \mapsto 1$ as $k \mapsto \infty$ as expected.

In order to compare our results with those given in [10], let us choose $N = 2$. Then, matrix Φ has the following form:

$$\Phi = \begin{pmatrix} 1 - \frac{im\lambda}{\hbar^2 k} & -\frac{im\lambda}{\hbar^2 k} e^{ik|a_1 - a_2|} \\ -\frac{im\lambda}{\hbar^2 k} e^{ik|a_1 - a_2|} & 1 - \frac{im\lambda}{\hbar^2 k} \end{pmatrix} . \tag{28}$$

For a better comparison with [10], let us choose $a_1 = -a$ and $a_2 = a$ with $a > 0$. Then,

$$\Phi^{-1} = \frac{1}{\det \Phi} \begin{pmatrix} 1 - \frac{im\lambda}{\hbar^2 k} & \frac{im\lambda}{\hbar^2 k}\, e^{i2ka} \\ \frac{im\lambda}{\hbar^2 k}\, e^{i2ka} & 1 - \frac{im\lambda}{\hbar^2 k} \end{pmatrix} , \tag{29}$$

with

$$\det \Phi = 1 - \frac{2im\lambda}{\hbar^2 k} + \frac{m^2\lambda^2}{\hbar^4 k^2} \left(e^{4ika} - 1 \right) . \tag{30}$$

These formulae are necessary to construct $\psi_k^+(x)$ as in equation (12) for $N = 2$. All scattering features can be obtained through this wave function. In particular, we may obtain the reflection and transmission coefficients. The wave function (12) reads for $x < -a$:

$$\begin{aligned} \psi_k^+(x) = e^{ikx} &+ \frac{im\lambda}{\hbar^2 k}\, e^{-ik(x+a)}\, \Phi_{11}^{-1}\, e^{-ika} + \frac{im\lambda}{\hbar^2 k}\, e^{-ik(x+a)}\, \Phi_{12}^{-1}\, e^{ika} \\ &+ \frac{im\lambda}{\hbar^2 k}\, e^{-ik(x-a)}\, \Phi_{21}^{-1}\, e^{-ika} + \frac{im\lambda}{\hbar^2 k}\, e^{-ik(x-a)}\, \Phi_{22}^{-1}\, e^{ika} . \end{aligned} \tag{31}$$

Then, from Eq. (23), we explicitly find the reflection amplitude

$$r(k) = (\det \Phi)^{-1} \frac{im\lambda}{\hbar^2 k} \left[\left(1 - \frac{im\lambda}{\hbar^2 k} \right) [e^{-2ika} + e^{2ika}] + 2 \left(\frac{im\lambda}{\hbar^2 k} \right) e^{2ika} \right] . \tag{32}$$

The values of k for which $T(k) = 1$ are known as *transmission resonances* in the literature [8]. One can plot the graph of T as a function of k and read the transmission resonances, as shown in the top right part of Fig. 2 for $N = 2$. To find explicitly these values, we can equivalently find the roots of the transcendental equation $r(k) = 0$ numerically. It has been shown in [10] that the energies corresponding to the transmission resonances are different from the resonance energies obtained from the poles of the S matrix or transmission coefficient.

The transmission coefficient for the Dirac delta potentials located periodically in the positive real axis is depicted for different numbers of N in Figure 2. This illustrates the appearance of the band gaps as we increase the number of centers, which was first shown in [30].

4 Threshold Anomaly

The threshold anomaly occurs for potentials consisting of N (≥ 2) Dirac delta potentials. We start to analyse the threshold anomalies for two Dirac delta centers by investigating $R(k)$ for small values of k. To this end, we expand it around $k = 0$:

$$R(k) = \left| -1 + \frac{i(-1 + \frac{8a^2m^2\lambda^2}{\hbar^4})}{2m\lambda(-1 + \frac{2ma\lambda}{\hbar^2})}\, \hbar^2 k + O(k^2) \right|^2 \tag{33}$$

It is easy to see that $R(k) \to 1$ as $k \to 0$, unless $\frac{2ma\lambda}{\hbar^2} = 1$. This means that the reflection probability is getting closer and closer to one as the energy of the incoming particles decreases, except for the critical case $\frac{2ma\lambda}{\hbar^2} = 1$. This is the generic case, and can be seen from Fig. 2. To understand the behavior of R near $k = 0$ in the critical case, we first substitute $a = \frac{\hbar^2}{2m\lambda}$ into $R(k)$ ($r(k)$ is given in Eq.(32)), and then expand it near $k = 0$ so that

$$R(k) = \left| \frac{4ia}{3} k + \frac{32a^2}{9} k^2 + O(k^3) \right|^2 . \tag{34}$$

This shows that the probability of reflection of the particle vanishes as the kinetic energy of the incoming particles goes to zero. This phenomenon is known as the threshold anomaly and has been first discussed in [7]. Actually, this fact can be seen more transparently by plotting the reflection coefficient as a function of a near $k = 0$.

As can be seen from Figure 3, the reflection coefficient sharply drops to zero at exactly the same critical value $a = \hbar^2/2m\lambda$. This is due to the appearance of a second bound state at this critical value. Note that this is exactly the same condition for the formation of the second bound state, as discussed in our recent paper [31]

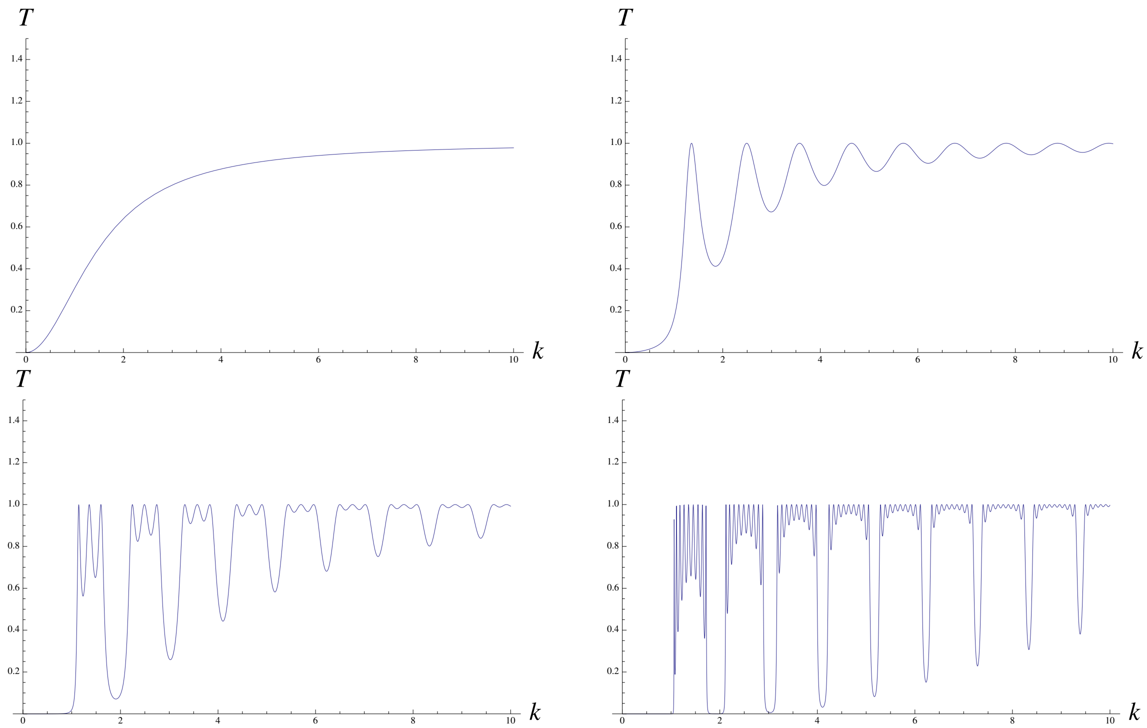

Figure 2: The transmission coefficient as a function of k for $N = 1, 2, 4, 10$, respectively. Here, $\lambda_i = 2$ and $|a_i - a_j| = 3$ for all i, j. We use the units such that $\hbar = 2m = 1$.

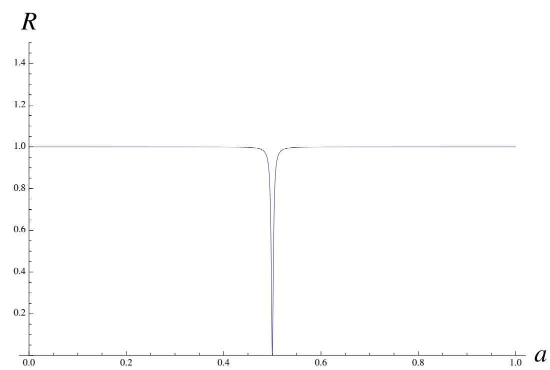

Figure 3: The reflection coefficient as a function of a for two centers. Here, $\lambda_1 = \lambda_2 = 2$ and $k = 0.01$ ($\hbar = 2m = 1$).

(the only difference is that the centers are separated by a in there). In other words, the underlying reason of this is the appearance of a bound state very close to the threshold energy [7].

For $N = 4$ case, the reflection coefficient near $k = 0$ is

$$R(k) = \left| -1 + \frac{i\left(384a^4m^4\lambda^4 - 512a^3m^3\lambda^3\hbar^2 + 160a^2m^2\lambda^2\hbar^4 - \hbar^8\right)}{4m\lambda\left(2am\lambda - \hbar^2\right)\left(8a^2m^2\lambda^2 - 8am\lambda\hbar^2 + \hbar^4\right)}\, k + O(k^2) \right|^2 . \tag{35}$$

Similar to the $N = 2$ case, $R(k) \to 1$ as $k \to 0$, unless the denominator is zero, that is,

$$\begin{aligned} 2am\lambda - \hbar^2 &= 0 \\ \left(8a^2m^2\lambda^2 - 8am\lambda\hbar^2 + \hbar^4\right) &= 0 . \end{aligned} \tag{36}$$

The solution to these equations are

$$m\lambda a = \left\{ \frac{\hbar^2}{4}\left(2 - \sqrt{2}\right), \frac{\hbar^2}{2}, \frac{\hbar^2}{4}\left(2 + \sqrt{2}\right) \right\} , \tag{37}$$

If we first substitute these solutions to $R(k)$ and then expand it, we obtain

$$R(k) = \begin{cases} \left| \dfrac{8iak}{3} + O(k^2) \right|^2 & \text{when } m\lambda a = \frac{\hbar^2}{2} \ , \\ \left| -\dfrac{4}{3} i \left(-3a + \sqrt{2}a \right) k + O(k^2) \right|^2 & \text{when } m\lambda a = \frac{\hbar^2}{4} \left(2 - \sqrt{2} \right) \ , \\ \left| \dfrac{4}{3} i \left(3a + \sqrt{2}a \right) k + O(k^2) \right|^2 & \text{when } m\lambda a = \frac{\hbar^2}{4} \left(2 + \sqrt{2} \right) \ . \end{cases} \tag{38}$$

This shows the threshold anomaly for $N = 4$ case. One can also see from Fig. 4 the vanishing behaviour of the reflection coefficient at the above critical cases near $k = 0$. All those critical values of a for which R vanishes

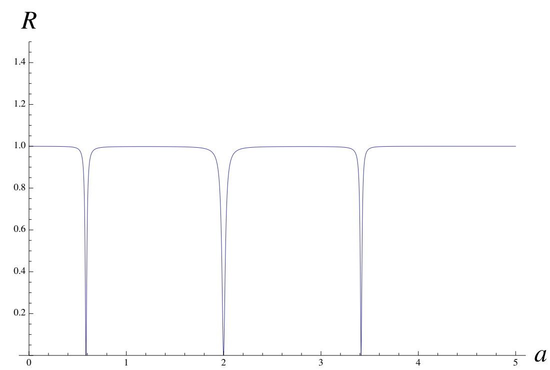

Figure 4: The reflection coefficient as a function of a for four centers. Here, $\lambda_1 = \lambda_2 = 1/2$ and $k = 0.01$ ($\hbar = 2m = 1$).

near $k = 0$ are just the critical values of the parameters in the model where the new bound states appear. In order to show this, we plot the flow of the eigenvalues of the principal matrix (see Eq. (A-2) in Appendix A) as a function of $|E|$, as shown in Fig. 5 by fixing the value of the parameter $a = 1$. The top left graph shows the critical situation $m\lambda a = \frac{\hbar^2}{4}\left(2 - \sqrt{2}\right)$, where the second bound state appears. Similarly, the other two graphs show the critical cases $m\lambda a = \frac{\hbar^2}{4}\left(2 + \sqrt{2}\right)$ and $m\lambda a = \frac{\hbar^2}{2}$, respectively. It is easy to notice that all the critical values for the appearance of the new bound states correspond exactly to the values of the parameter where the threshold anomaly occurs.

All these show that the method that we have used is very useful and systematic for large values of centers whereas the standard method may become very cumbersome in dealing with more than two centers.

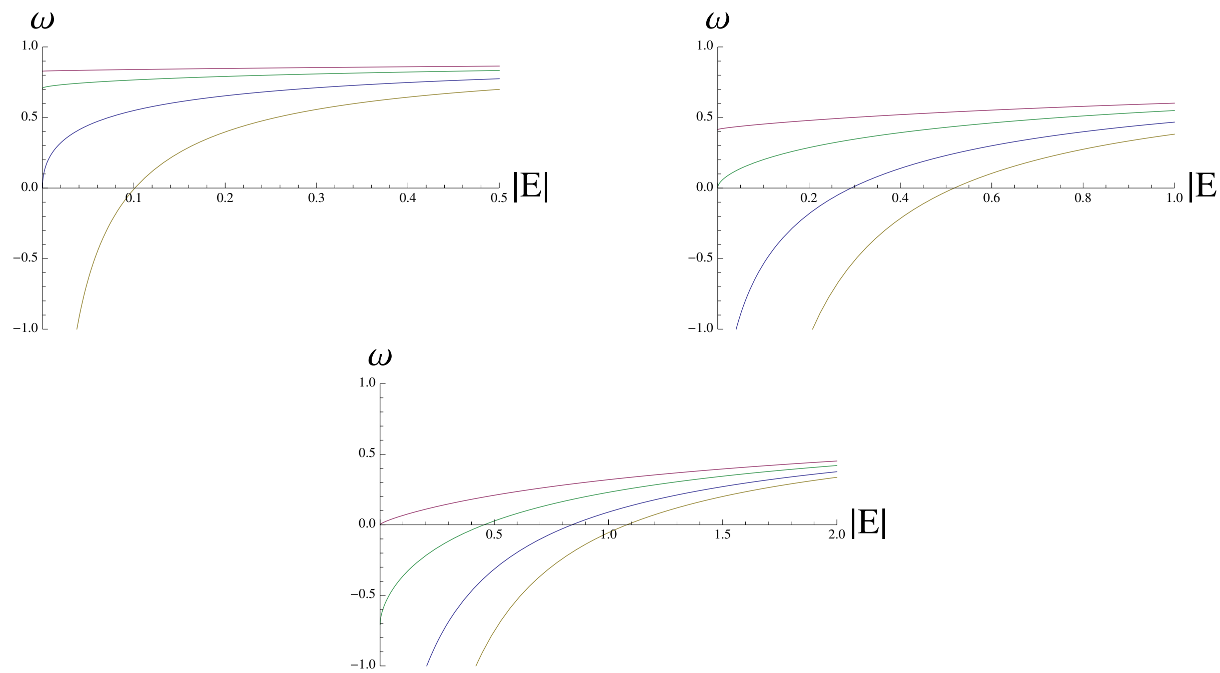

Figure 5: Eigenvalues of the principal matrix Φ for the critical values of the parameters ($\hbar = 2m = 1$). We choose $a = 1$.

5 Resonances and Gamow states

Models with two Dirac delta potentials in the context of resonances have been discussed for instance in [14, 17] and see references therein. We recall that resonances are always produced by a perturbation on the free Hamiltonian. In other words, in order to have resonances, we need a Hamiltonian pair (H_0, H), where H_0 is "free" or unperturbed and $H = H_0 + V$, the total Hamiltonian. In our case, the perturbation is given by multiple Dirac delta potential V.

Let us emphasize a very important point about one dimensional scattering, that has been previously mentioned. Concerning resonances and perfect transmission values, a certain confusion arises in the literature, see for example [6]. For some types of one-dimensional potentials there exist values of the energy for which the transmission coefficient is equal to one. They are sometimes called resonances or transmission resonances. In [10], a terminology - *perfect transmission* - is proposed to describe this phenomenon, but we will stick to *transmission resonances*. On the other hand, we shall reserve the name of resonance for a type of the poles of the scattering S matrix. If the S-matrix is written in terms of its dependence on the momentum k of the incident particle, $S(k)$, and satisfies some general assumptions, then it admits an analytic continuation to the complex values of k. Then resonances are characterized by pairs of poles of $S(k)$ located in the lower half plane symmetrically with respect to the imaginary axis. These pairs of poles reveal the existence of quantum unstable states *or* resonances, both terms denote the same physical reality. One can find a deep and thoroughly study of this in [32, 33].

Nevertheless, the poles of the transmission coefficient coincide with the poles of the scattering S matrix [34]. Due to this fact, resonance poles can be calculated by using the transcendental equation $\det \Phi = 0$. We may find four types of solutions:

1.- Simple poles in the positive imaginary k-axis. They have the form $i\alpha$, with $\alpha > 0$. They are associated with the bound states [33].

2.- Simple poles in the negative imaginary k-axis. They have the form $-i\alpha$, with $\alpha > 0$. Its physical meaning is not always clear [35, 36, 37]. They are associated with the states called *antibound* or *virtual* states [32, 33].

3.- A possible pole at the origin. This may be associated with the situation in which causality conditions, as usually stated, do not hold [32].

4.- Pairs of poles of the form $\pm k_0 - ik_1$ with $k_0, k_1 > 0$. Each pair of poles of this kind represents a resonance [32, 33]. In principle, these poles may have any (finite) multiplicity, although for realistic models this multiplicity is one. The number of resonance pairs of poles in systems with finite range potentials (the potential is zero outside a bounded region) is infinite.

The method used in [10] is based on the usage of the continuity and jump conditions of the wave function and its derivative at the location of the Dirac delta centers, respectively. In contrast, we adopt Lippmann-Schwinger equation to find the scattering and resonance information for the system. In particular, for $N = 2$, the equation $\det \Phi = 0$, where $\det \Phi$ is given by (30) is identical to the formula (28) in [10] if we identify a in our equations with $a/2$ and $-\lambda$ with $\nu_1 = \nu_2$ in equation (28) in [10]. Therefore, we conclude that the results in [10] for the scattering states and resonances are consistent with our results. Note that in [10], the locations of the resonance poles are given in terms of the complex energies. These complex energies are calculated using the formula $E = \hbar^2 k^2/2m$, so that if $k = \pm k_0 - ik_1$, then $E \pm i\hbar\Gamma/2 = (\mp k_0 - ik_1)^2$. The real part E is called the resonant energy and the imaginary part is related to the mean life of the resonance [33].

At this point, we need to remark that the transformation $E := \hbar^2 k^2/2m$ transforms the function $S(k)$ into a function $S(E)$, which is now defined in a two-sheeted Riemann surface, where each sheet is a complex plane, see [33]. In this case, resonance poles are complex conjugate poles located on the second sheet at the points $E \pm i\hbar\Gamma/2$, with E, $\Gamma > 0$. Both complex conjugate poles represent the same resonance.

By definition a Gamow state ψ is an eigenvector (wave function) of the total Hamiltonian $H = H_0 + V$ having the complex eigenvalue, $H\psi = (E - i\Gamma/2)\psi$, where $E - i\Gamma/2$ is called the resonance pole. Then, for Gamow wave functions ψ we have

$$e^{-\frac{i}{\hbar}tH}\psi = e^{-\frac{i}{\hbar}Et}e^{-\Gamma t/2}\psi\,, \tag{39}$$

so that ψ decays exponentially with time. For this reason, Gamow wave functions may be looked as state wave functions for resonances.

However, we have two problems for this interpretation. The former has to do with the self-adjointness of the Hamiltonian H. A self-adjoint Hamiltonian cannot have complex eigenvalues in a Hilbert space. The only possible solution is to extend the Hilbert space to a larger space with not normalizable wave functions so that the equation $H\psi = (E - i\hbar\Gamma/2)\psi$ as well as Equation (39) make sense in this larger space. This has been done with the help of the rigged Hilbert spaces, a mathematical tool that was initially used to introduce a rigorous presentation of the Dirac formalism for quantum mechanics [21, 23, 24, 25, 26]. Note that we represent the resonance by one of the resonance poles $E - i\Gamma/2$. The other one $(E + i\hbar\Gamma/2)$ will play a symmetric role which will go beyond the scope of the present paper.

The second difficulty comes from the fact that it is not clear that quantum decaying systems decay exponentially for all times. In any case, experiments have shown that exponential decay is a very good approximation for decay behavior for essentially all ranges of time, with the possible exception of very short times or very large times. Thus, Gamow wave functions can be good approximations for wave functions of decaying states for the majority values of time. In our case, being given a resonance defined by a pair of poles of the S matrix, we may construct its Gamow wave function. The method is to use an analytic continuation of equation (2) and we shall use a description of it. Technicalities can be found in [38, 39]. Let $E_R - i\hbar\Gamma/2$ be the location of a resonance pole in the energy representation. The analytic continuation of (2) at the complex value k_R so that $z_R := E_R - i\hbar\Gamma/2 = k_R^2\hbar^2/2m$ is given by

$$|k_R^+\rangle = |k_R\rangle - G_0(z_R)V|k_R^+\rangle\,. \tag{40}$$

where $|k_R^+\rangle$ and z_R are the eigenvectors and eigenvalues of H, respectively:

$$H|k_R^+\rangle = \frac{k_R^2\hbar^2}{2m}\,|k_R^+\rangle = z_R|k_R^+\rangle \tag{41}$$

Thus, $|k_R^+\rangle$ is the Gamow vector for the resonance with resonance pole k_R. This Gamow vector in the coordinate representation is $\psi_R(x) := \langle x|k_R^+\rangle$, so that

$$(H\psi_R)(x) = \langle x|H|k_R^+\rangle = z_R\langle x|k_R^+\rangle = z_R\psi_R(x)\,. \tag{42}$$

If we use $V = -\sum_{i=1}^N \lambda_i|a_i\rangle\langle a_i|$ and multiply (40) from the left by $\langle x|$, we obtain:

$$\langle x|k_R^+\rangle = \langle x|k_R\rangle + \sum_{i=1}^N \lambda_i\langle x|G_0(z_R)|a_i\rangle\langle a_i|k_R^+\rangle\,. \tag{43}$$

Let us write the complex number k_R in terms of its real and imaginary parts as $k_R = k_r - ik_I$. Since $\langle x|k_R\rangle = e^{ik_Rx}$ by the process of analytic continuation, equation (43) becomes:

$$\psi_R^+(x) = e^{ik_rx}\, e^{k_Ix} + \sum_{i=1}^{N} \lambda_i G_0(x, a_i; z_R)\, \psi_R^+(a_i)\,. \tag{44}$$

Proceeding as in Section 2, we can find $\psi_R^+(a_i)$ so that

$$\psi_R^+(x) = e^{ik_rx}\, e^{k_Ix} + \sum_{i=1}^{N}\sum_{j=1}^{N} \frac{im\sqrt{\lambda_i\lambda_j}}{\hbar^2(k_r+ik_I)}\, e^{i(k_r+ik_I)|x-a_i|}\, [\Phi^{-1}(z_R)]_{ij}\, e^{i(k_r+ik_I)a_j}\,. \tag{45}$$

We now observe that the first term in the right hand side of (44) diverges exponentially as $x \longmapsto \infty$. In the second term, we have a sum including the Green function for the free Hamiltonian H_0, given by

$$G_0(x, a_j; z_R) = \frac{im}{\hbar}\, \frac{\exp\{\frac{i}{\hbar}\sqrt{2mz_R}|x-a_j|\}}{\sqrt{2mz_R}} = \frac{im}{\hbar}\, \frac{\exp\{\frac{i}{\hbar}\sqrt{2m}\, k_r|x-a_j|\}\exp\{\frac{1}{\hbar}\sqrt{2m}\, k_I|x-a_j|\}}{\sqrt{2mz_R}}\,. \tag{46}$$

Again since k_I is positive, we observe an exponential behavior for large values of $|x|$. The conclusion is that Gamow wave functions cannot be normalized in the sense of square integrability, but contrary to Dirac kets or plane waves which are bounded but not square integrable, they show exponential behavior at the infinity in the coordinate representation. This behavior was sometimes called the spatial or exponential catastrophe. With a proper interpretation of Gamow wave functions in terms of generalized functions in rigged Hilbert spaces, one may show that this is far from being a catastrophe [39].

6 Virtual States for $N = 2$

In this short section, we summarize the results how the location of the poles of the transmission coefficient (or S -matrix) change with respect to the distance between two attractive Dirac delta potentials within our formalism. As previously emphasized, the poles of the transmission coefficients are given by the solution of the transcendental equation $\det \Phi(k) = 0$.

Here we choose that $a_1 = 0$ and $a_2 = a$, and the units such that $\hbar = 2m = 1$. Then, the complex solutions of $\det \Phi(E_k + i0) = 0$ can be found in the lower half plane of the complex k plane. In order to follow the motion of these poles, we plot the zero level curves of $\Re(\det \Phi(E_k + i0))$ (blue curves in Figure 6) and $\Im(\det \Phi(E_k + i0))$ (red curves in Figure 6) by fixing λ for different values of a. The intersections of the red and blue curves on the complex k plane are the solutions of $\det \Phi(E_k + i0) = 0$. The simple poles on the positive imaginary k

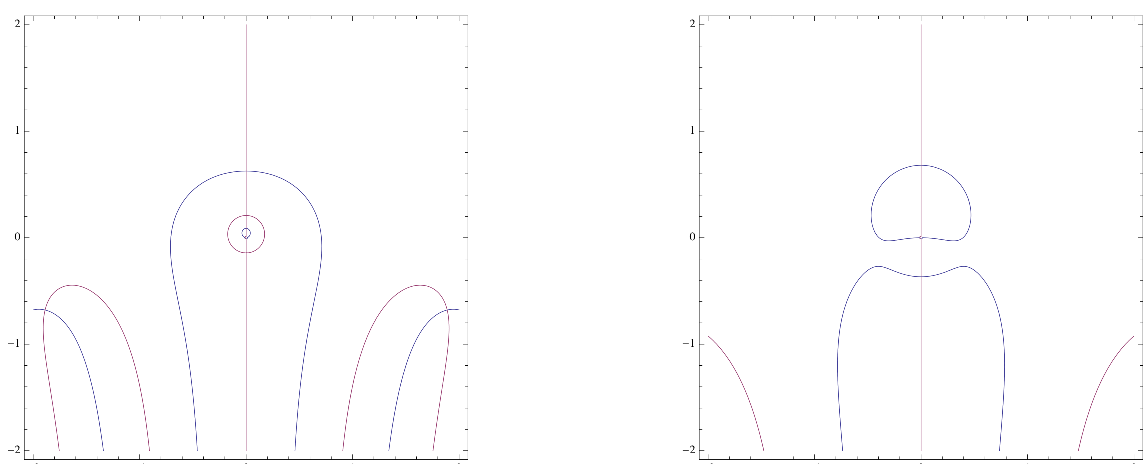

Figure 6: Contour plots of the $\Re(\det \Phi)$ and $\Im(\det \Phi)$ for $a = 2.2$ on the left and $a = 1.5$ on the right. $\lambda_1 = \lambda_2 = 1$ in both cases.

axis correspond to the bound states, whereas the ones in the negative imaginary k axis are known as virtual states [20]. As emphasized in [31], it is well known that there are two bound states when a is sufficiently large ($a > \hbar^2/m\lambda$ or the critical case $a = 2$ for particular choice of the parameter $\lambda = 2$) and the second bound state eventually becomes a virtual state as we decrease the distance between the centers. From Fig. 6, if the distance between the centers is $d = 2a = 1.4$, the second bound state pole is shifted to the negative imaginary axis. Thus, it becomes a virtual state. This phenomenon also occurs for some other potentials as well, e.g., rectangular well and barrier potentials [40, 41].

7 Conclusion

Systems of N contact potentials, particularly if these potentials are linear combinations of Dirac deltas are usually solvable systems suitable to study important features in non-relativistic quantum mechanics such as bound states, scattering transmission and reflection coefficients, threshold anomalies, resonances as quantum unstable states and virtual states (also called anti-bound states). In this study, we have shown that the Lippmann-Schwinger equation in momentum space is a very appropriate tool to perform calculations in order to find properties of the above mentioned quantum features. In the case of N Dirac deltas, we have found explicitly the solution of the Lippmann-Schwinger equation in terms of the matrix Φ, which encodes all the information about the system. This method allows us to discuss the scattering (and bound states as well [31]) problem for arbitrary number of centers without solving the system of equation from the boundary conditions imposed at the location of Dirac delta centers and this substantially simplifies the calculations. Therefore, we were able to investigate transmission and reflection probabilities, threshold anomalies for $N > 2$ delta centers. Although we have explicitly found the scattering information about a very particular model, where a single particle interacts with finitely many singular potentials described formally by Dirac delta functions, it can be applied to the other systems as well by modelling them by a special arrange of the Dirac delta potentials (see [5]). Hence, the methodology we have used here is of a general character.

8 Appendix A: Bound States for N Dirac Delta Potentials

As we have mentioned in the introduction, the Dirac delta potentials can be represented by projections given by Eq.(4). Then, it is a simple exercise to show that the Schrödinger equation can be put into a matrix equation

$$\sum_{j=1}^{N} \Phi_{ij}(E)\psi(a_j) = 0 \, , \tag{A-1}$$

where

$$\Phi_{ij}(E) = \begin{cases} 1 - \dfrac{m\lambda_i}{\hbar\sqrt{2m|E|}} & \text{if } i = j \, , \\[2ex] -\dfrac{m\sqrt{\lambda_i\lambda_j}}{\hbar\sqrt{2m|E|}} \exp\left(-\sqrt{2m|E|}|a_i - a_j|/\hbar\right) & \text{if } i \neq j \, . \end{cases} \tag{A-2}$$

Here E is real and negative. Actually, the matrix Φ given in Eq.(22) is exactly the analytical continuation of the above matrix Φ. The bound state energies can be found from the non-trivial solution of the matrix equation for Φ, that is, the bound state energies must satisfy $\det \Phi(E) = 0$. This was explicitly shown in our recent paper [31]. Moreover, one can also imagine the following eigenvalue problem for the matrix Φ, i.e.,

$$\Phi(E)A(E) = \omega(E)A(E) \, . \tag{A-3}$$

Then, the bound state energies are the zeroes of the eigenvalues ω. This tells us that the eigenvalues of the *linear* Schrödinger equation $H\psi(x) = E\psi(x)$ are obtained through a *non-linear* transcendental algebraic problem, $\omega(E) = 0$.

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