Two channel scattering Problem with Arbitrary coupling.

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The present work deals with the calculation of transition probability between two diabatic potentials coupled by any arbitrary coupling. The method presented in the manuscript is applicable to any type of coupling but for numerical calculations we have assumed the arbitrary coupling as Gaussian coupling. This arbitrary coupling is expresses as a collection of Dirac Delta functions and by the use of transfer matrix technique the transition probability from one diabatic potential to another diabatic potential is calculated. We examine our approach by considering the case of two constant potentials coupled by Gaussian coupling as an arbitrary coupling.

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I. INTRODUCTION

The solution of the time-independent Schrödinger equation using numerical methods is of keen interest in early days of quantum mechanics\cite{1}. There is a very limited number of potentials which can be analytically solvable for wavefunctions to calculate the reflection as well as transmission amplitudes\cite{2}. Various physical problems in interdisciplinary sciences do not allow simple solutions in the format of Schrödinger equation, hence in such cases the Schrödinger equation is solved numerically\cite{3} or by taking approximations of the potential under consideration by using the solvable one\cite{4, 5} or different methods like factorization\cite{6, 7}, the path integral\cite{8}, eigen value momentum method\cite{9} and power series expansion method\cite{10} along with many more available in the literature. Present manuscript also deals with such methods in which an arbitrary potential is expressed by Dirac delta potentials. Use of Dirac delta potentials to model potential barriers has a long history when Kronig and Penney\cite{11} modeled the equidistant rectangular barriers by such functions to understand the quantum mechanics of electrons in crystal lattices. Such kind of models were also used to study the absorption spectra of organic dyes\cite{12}. Existence of Surface states is also predicted by the use of such models as reported by Tamm\cite{13}. Saxon and Hunter\cite{14} expressed the atomic fields by Dirac delta potentials and derived the wavefunctions and energy levels for monoatomic and diatomic Kronig-Peney models. Frost also reported in his findings the models of hydrogen like atoms\cite{15}, hydrogen-molecule ion\cite{16} and more complex systems\cite{17} by making use of single and multiple Dirac delta potentials. These citations in the literature for the use of Dirac delta potentials proved it to be useful as an analytical solvable model in variety of applications involving novel concepts of physics. We have also explored the area of non-adiabatic transitions using analytical methods (Dirac Delta coupling model) and reported analytical solution in those cases where two or more arbitrary potentials are coupled by Dirac Delta interactions\cite{18-23}. This Dirac Delta function coupling model has a plus point that we can get exact analytical solution using such model. Recently we have extended our research to deal with the cases where two potentials are coupled by an arbitrary interaction\cite{24}. In our most recent paper it is shown that if we use Dirac Delta coupling model, it is possible to express N-channel problem by N independent ‘single’ channel problem and hence one can have a realistic solution of multi-channel scattering problem. Using the same model it is shown that transition probability from first diabatic potential to any other potential can be easily calculated by using single equation with two boundary conditions. We have also reported extension of two state scattering problem to three state scattering problem where we have to find the six boundary conditions and with the help of these six boundary conditions we can calculate the transition probability from one diabatic potential to another diabatic potential by the use of a simple analytical formula. The present manuscript deals with the case in which there is arbitrary coupling between the two state and this arbitrary coupling is expressed as a collection of Dirac delta function potentials and hence the transition probability form one diabatic state to another state is calculated by using transfer matrix method.

II. METHOD

The main idea behind this study is to express a potential as a sum of Dirac delta potentials i.e.

\[
V(x) = \int_{-\infty}^{\infty} e^{-\alpha x^2} = \sum_{N=1}^{n} K_n \delta(x - x_n)
\]  

(1)

In the above equation a smooth potential represented by Gaussian function is expressed by a sum of Dirac delta functions. \(x_n\) represents the position of the dirac delta function and \(K_n\) represents the strength of the delta function. The schematic diagram representing the problem is given in Figure 1. This method is applicable to any kind of coupling where the area under the coupling is represented as a sum of areas of the Dirac delta potentials used to express the coupling along with the discretization scheme used.

III. TWO STATE SCATTERING

We consider a particle moving on any of the two diabatic curves and our problem defines the calculation of transition probability of the particle to be still on that diabatic curve after time \(t\). We write the probability amplitude for the particle as

\[
\Psi(x) = \begin{pmatrix}
\psi_1(x) \\
\psi_2(x)
\end{pmatrix}
\]  

(2)
where \( \psi_1(x) \) and \( \psi_2(x) \) are the probability amplitude for the two states. The Hamiltonian is given by

\[
H = \begin{pmatrix}
H_{11}(x) & V_{12}(x) \\
V_{12}(x) & H_{22}(x)
\end{pmatrix},
\]

(3)

where \( H_{11}(x) \), \( H_{22}(x) \) and \( V_{12}(x) \) are defined by

\[
H_{11}(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V_1(x),
\]

(4)

\[
H_{22}(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V_2(x) \quad \text{and} \quad
V_{12}(x) = V_{21}(x) = V(x).
\]

The above \( V_1(x) \) and \( V_2(x) \) are determined by the shape of that diabatic curve. \( V(x) \) is a coupling function which is a Gaussian function as discussed in section 2, and is approximated as a collection of Dirac Delta potentials. The time-independent Schrödinger equation is written in the matrix form and the equations given below are derived for the general position of the Dirac delta potential at \( x = x_n \).

\[
\begin{pmatrix}
H_{11}(x) & V_{12}(x) \\
V_{12}(x) & H_{22}(x)
\end{pmatrix}
\begin{pmatrix}
\psi_1(x) \\
\psi_2(x)
\end{pmatrix}
= E
\begin{pmatrix}
\psi_1(x) \\
\psi_2(x)
\end{pmatrix}.
\]

(5)

This is equivalent to

\[
H_{11}(x)\psi_1(x) + K_n \delta(x - x_n)\psi_2(x) = E\psi_1(x) \quad \text{and} \quad
K_n \delta(x - x_n)\psi_1(x) + H_{22}(x)\psi_2(x) = E\psi_2(x).
\]

(6)

Integrating the above two equations from \( x_n - \eta \) to \( x_n + \eta \) (where \( \eta \to 0 \)) we get the following two boundary conditions

\[
-\frac{\hbar^2}{2m} \left[ \frac{d\psi_1(x)}{dx} \right]_{x_n-\eta}^{x_n+\eta} + K_n\psi_2(x_n) = 0 \quad \text{and} \quad
-\frac{\hbar^2}{2m} \left[ \frac{d\psi_2(x)}{dx} \right]_{x_n-\eta}^{x_n+\eta} + K_n\psi_1(x_n) = 0.
\]

(7)

Also we have two more boundary conditions

\[
\psi_1(x_n - \eta) = \psi_1(x_n + \eta) \quad \text{and} \quad
\psi_2(x_n - \eta) = \psi_2(x_n + \eta).
\]

(8)

Using the above four boundary conditions we derive the transition probability from one diabatic potential to the other coupled by arbitrary coupling and this arbitrary coupling is expressed as a sum of Dirac Delta function potentials. In region 1 \((x < x_n)\), the time-independent Schrödinger equation for the first potential is given by

\[
-\frac{1}{2m} \frac{\partial^2 \psi_1(x)}{\partial x^2} + V_1(x)\psi_1(x) = E\psi_1(x).
\]

(9)

The above equation has the following solution

\[
\psi_1(x) = A_n e^{ik_1 x} + B_n e^{-ik_1 x},
\]

(10)

where \( k_1 = \sqrt{\frac{2m}{\hbar^2}(E - V_1)} \). In region 2 \((x > x_n)\), the time-independent Schrödinger equation for the first potential is given by

\[
-\frac{1}{2m} \frac{\partial^2 \psi_1(x)}{\partial x^2} = E\psi_1(x)
\]

(11)

Physically acceptable solution of the above equation is given by

\[
\psi_1(x) = A_{(n+1)} e^{ik_1 x} + B_{(n+1)} e^{-ik_1 x}.
\]

(12)

In region 1 \((x < x_n)\), the time independent Schrödinger equation for the second potential is given by

\[
-\frac{1}{2m} \frac{\partial^2 \psi_2(x)}{\partial x^2} + V_2\psi_2(x) = E\psi_2(x).
\]

(13)
Physically acceptable solution is given by

\[ \psi_2(x) = D_n e^{ik_2x} + F_n e^{-ik_2x}, \]

where \( k_2 = \sqrt{\frac{2m}{\hbar^2} (E - V_2)} \). In region 2 \( (x > x_n) \), the time-independent Schrödinger equation for the second potential is given by

\[ -\frac{1}{2m} \frac{\partial^2 \psi_2(x)}{\partial x^2} + V_2 \psi_2(x) = E \psi_2(x). \]

Physically acceptable solution is given by

\[ \psi_2(x) = D_{(n+1)} e^{ik_2x} + F_{(n+1)} e^{-ik_2x}. \]

In considering the smooth Gaussian potential expressed by a collection of Dirac Delta potentials the wavefunction between two consecutive Dirac Delta potentials is a free particle wavefunction and is given as

\[ \psi_n(x) = A_n e^{ik_1x} + B_n e^{ik_1x}, \]

where \( \psi_n(x) \) is the wavefunction between the \( n^{th} \) and \( (n + 1)^{th} \) Dirac Delta functions. \( \hbar k_1 = \sqrt{2m(E - V_1)} \) is the wave momentum. At the position of \( \delta \) functions, the given wavefunction has to satisfy the boundary conditions as mentioned in equations no (7) and (8). These boundary conditions will give us a general \( (4 \times 4) \) matrix for location of the \( \delta \) function at \( x_n \) as given below

\[ T_n = \begin{bmatrix}
1 & 0 & \frac{-ie^\sqrt{2x-a_n}n\delta - ie^\sqrt{2x+a_n}k[n]}{\sqrt{2k_1}} & \frac{-ie^\sqrt{2x-a_n}n\delta - ie^\sqrt{2x+a_n}k[n]}{\sqrt{2k_1}} \\
0 & 1 & \frac{-ie^{-\sqrt{2x-a_n}n\delta + ie^\sqrt{2x+a_n}k[n]}}{\sqrt{2k_1}} & \frac{-ie^{-\sqrt{2x-a_n}n\delta + ie^\sqrt{2x+a_n}k[n]}}{\sqrt{2k_1}} \\
\frac{-ie^{\sqrt{2x-a_n}n\delta + ie^{-\sqrt{2x+a_n}k[n]}}}{\sqrt{2k_1}} & \frac{-ie^{\sqrt{2x-a_n}n\delta + ie^{-\sqrt{2x+a_n}k[n]}}}{\sqrt{2k_1}} & 1 & 0 \\
\frac{-ie^{-\sqrt{2x-a_n}n\delta + ie^{\sqrt{2x+a_n}k[n]}}}{\sqrt{2k_1}} & \frac{-ie^{-\sqrt{2x-a_n}n\delta + ie^{\sqrt{2x+a_n}k[n]}}}{\sqrt{2k_1}} & 0 & 1 
\end{bmatrix} \]

The total transfer matrix can be considered as the multiplication of all transfer matrices \( T_n \),

\[ T = T_{n+1}T_n \ldots \ldots T_1T_0. \]

The transmission coefficient and reflection coefficient across each transfer matrix is equal to 1 and same is true for general matrix i.e.

\[ |T|^2 + |R|^2 = 1 \]

The transition probability from one diabatic potential to another diabatic potential coupled by arbitrary potential (Gaussian potential expressed by a sum of Dirac Delta potentials is expressed as

\[ T_{12} = 1 - |T|^2 - |R|^2 \]

In the above equation \( T_{12} \) represents the transition probability from one diabatic potential to another diabatic potential. We calculated the transition probability for this arbitrary coupling as a collection of \( N \) Dirac delta functions where \( N = n \) can be any number but in the current work \( n = 1, 3, 5, 7, 9, 13, 15 \) and \( 21 \) before the convergence reaches for 21 number of Dirac Delta functions. Hence our arbitrary coupling is best expressed by a collection of 21 Dirac delta functions. The Plots for transition probability for different number of Dirac Delta functions is represented in Figure 3 and 4 respectively.

**IV. CONCLUSIONS**

The present manuscript deals with the application of transfer matrix technique to the study of non adiabatic transitions or curve crossing problems. The two diabatic constant potentials are coupled by an arbitrary coupling and the transition probability from one diabatic potential to another is calculated. The arbitrary coupling can be any type of coupling but in the present case for numerical calculations we have chosen the Gaussian coupling which is expressed by a collection of Dirac delta potentials. The result of our calculation are shown in Figure 3 and Figure 4 respectively.
It is observed that as we increase the number of Dirac delta potentials the value of transition probability is decreasing and further converges when the coupling is expressed as a collection of 15, 17 and 21 Dirac delta potentials.

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