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Exact solution of Schrodinger equation for two state problem with time dependent coupling

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HIGHLIGHTS

- Exact analytical solution for SE with time dependent coupling is found.
- Dirac Delta coupling model is used.
- Strength of Dirac Delta has varied dependence on time.

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ABSTRACT

The present work focuses on the exact solution of the time dependent Schrodinger equation involving two potentials coupled by a time dependent Dirac Delta function potential. The problem involving the partial differential equations in two variables can be reduced to a single integral equation in Laplace domain and by knowing the wave function at the origin we can derive the wave function everywhere. Solutions for the different time variation of the strength of the Dirac Delta function potentials has been derived.

1. Introduction

There are very limited cases in which a time-dependent Schrodinger equation with a time dependent potential can be solved exactly. Some of the examples may include time dependent harmonic oscillator [1–3], infinite potential well with a moving boundary [4–6] and few more examples [7]. Two types of time-dependent problems which are commonly investigated include the simple scattering problem and the other one includes the Delta functional potential where strength varies with time. The first kind has a periodic dependence on time [8] and amounts to a steady state solution while the other type is solved using Floquet formalism [9]. There are also other time dependent scattering problems involving delta function potentials whose solutions are simple plane waves [7]. There also exist time dependent problems which are solved using diffusive solution to the Schrodinger wave equation. The majority of the work involving the time dependent potentials is solved by using delta or a rectangular barrier. Intrinsically time dependent processes such as quantum mechanical processes in a certain time dependent external field become very important these days because of remarkable progress of laser technology which means that laser intensity and frequency can be now designed as a function of time. Two kind of approaches are adopted by scientists to handle the time dependent problems. Out of these approaches one is path integral

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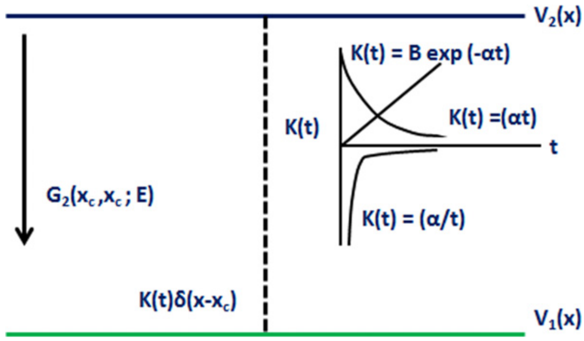

Fig. 1. Schematic view of our problem.

of Feynman type and other is Laplace Transforms. The main disadvantage of the former method is slow convergence which is rectified by introducing a rapidly converging scheme [10]. Our earlier work in this area was dedicated towards time independent coupling [11–17]. In the present work we developed a new approach of study of nonadiabatic transitions involving time dependent potentials coupled by time dependent Dirac Delta potential. In this work we focus on the problem involving two time independent potentials coupled by a time dependent Dirac Delta potential. Our problem involving the partial differential equations in two variables is reduced to a single integral equation in Laplace domain and by knowing the wave function at the origin we can derive the wave function everywhere. Solutions for the different time variation of the strength of the Dirac Delta potentials have been derived. Our time dependent model can be used to model the displacement of an atom with an STM tip. A delta function well can be used to model the STM potential at the vicinity of the end of the STM tip which moves uniformly and probability to remain trapped in the moving tip can be calculated. At zero time this well is localized at $x = 0$, however for time greater than zero the well moves at constant velocity v. The potential well can be considered as $V(x, t) = -k_0\delta(x)$ for $t \leq 0$ and $V(x, t) = -k_0\delta(x - vt)$ for $t > 0$.

2. Methodology

The schematic view of our problem is presented in Fig. 1. The two diabatic states are coupled to each other by a time dependent Dirac Delta function where the effect of second state is entering the first state in terms of Green's function. Strength of the Dirac delta function has varied dependence which includes the linear, inverse and exponential variation. We start with the case where two time dependent constant potentials are coupled to each other by a time dependent coupling. The Schrödinger equation in this case can be written as

$$\mathrm{i}\frac{\partial}{\partial t}\begin{bmatrix}\phi_1(x,t)\\ \phi_2(x,t)\end{bmatrix} = \begin{bmatrix}H_{11} & V_{12}\\ V_{21} & H_{22}\end{bmatrix}\begin{bmatrix}\phi_1(x,t)\\ \phi_2(x,t)\end{bmatrix}. \tag{1}$$

The above equation is equivalent to the following

$$\mathrm{i}\frac{\partial\phi_1(x,t)}{\partial t} = H_{11}\,\phi_1(x,t) + V_{12}\,\phi_2(x,t) \tag{2}$$

$$\mathrm{i}\frac{\partial\phi_2(x,t)}{\partial t} = H_{22}\,\phi_2(x,t) + V_{21}\,\phi_1(x,t),$$

if V_{12} and V_{21} are the coupling between the potentials represented by $V_{12} = V_{21} = 2k(t)\delta(x)$, then the above equations reduce to

$$\mathrm{i}\frac{\partial\phi_1(x,t)}{\partial t} = H_{11}\,\phi_1(x,t) + 2k(t)\delta(x)\,\phi_2(x,t) \tag{3}$$

$$\mathrm{i}\frac{\partial\phi_2(x,t)}{\partial t} = H_{22}\,\phi_2(x,t) + 2k(t)\delta(x)\,\phi_1(x,t).$$

Taking the Laplace transform of Eq. (3), it can be written as

$$H_{11}\,\overline{\phi_1}(x,s) + 2L[k(t)\delta(x)\phi_2(x,t)] = \mathrm{i}s\,\overline{\phi_1}(x,s) - \mathrm{i}\,\phi_1(x,0). \tag{4}$$

In a similar way other equation can also be written as

$$H_{22}\,\overline{\phi_2}(x,s) + 2L[k(t)\delta(x)\phi_1(x,t)] = \mathrm{i}s\,\overline{\phi_2}(x,s) - \mathrm{i}\,\phi_2(x,0). \tag{5}$$

In the next coming sections we will discuss the different cases in which the strength of the Dirac Delta function potential coupling the two states is varied in time and a solution for the single equation is obtained.

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