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Quantum shutter transient solutions and the delay time for the δ potential

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The analytical solution to the time-dependent Schrödinger equation for tunneling using cutoff plane-wave initial conditions is in general given by the sum of two types of terms that exhibit a transient behavior. The time evolution of the probability density for the δ potential is compared with the free case to investigate in this case the role of these transient terms for the delay time. We find, by a dynamical calculation, that the delay time arises from the interference between these transient terms and we show that at very long times it goes into the *phase delay time*, given by the energy derivative of the phase of the transmission amplitude.

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I. INTRODUCTION

It is well known that the notion of delay time originated more than 50 years ago in connection with scattering problems in nuclear physics [1,2]. This notion tell us that the action of a potential on a propagating quantum particle is to produce a delay time relative to the free propagating situation. At asymptotically long times one may obtain an expression for the delay time by using the time honored method of the stationary phase. In one dimension this corresponds to the derivative with respect to the energy of the phase θ of the transmission amplitude, namely $\tau_\theta = \hbar d\theta/dE$ [3]. We shall refer to this expression as the *phase delay time*. Clearly, since the transmission amplitude may be obtained solving the time-independent Schrödinger equation, it is not necessary to perform a time-dependent analysis to obtain the above expression [4,5]. In a dynamical analysis the delay time is obtained as the time difference between the maxima of the peaks of the transmitted and free evolving probability densities. We shall refer to the result of this calculation as the *dynamical delay time* and denote it by Δt. It requires to solve the time-dependent Schrödinger equation as an initial value problem. It has been customary to choose as initial state a Gaussian wave packet and solve numerically the time-dependent Schrödinger equation to get the transmitted and free wave packets in order to calculate Δt [6]. In contrast with this, as discussed below, our approach considers initially cutoff waves [7].

In recent work, an exact analytical solution to the time-dependent Schrödinger equation was obtained for cutoff initial plane waves impinging on a potential [8]. The dynamical problem may be visualized as a *gedanken experiment* consisting of a shutter, situated say at $x=0$, that separates initially a beam of particles from a potential barrier. At $t=0$, the shutter is opened and we follow the transmitted probability density as it evolves in time through $x>0$. One may envisage a whole class of problems whose dynamical description is closer to the above quantum shutter setup than scattering by a Gaussian wave packet [9]. In general, the transmitted solution exhibits two types of transient terms. At asymptotically long times one of them goes into the stationary solution to the problem, whereas the other tends to a vanishing value [8]. However, at finite times one may ask how these transient terms contribute to the delay time. In this work, we address the above question for the case of an exactly solvable model, namely the δ barrier potential. We investigate the *dynamical delay time* Δt for that potential. Since at long times the transient solutions go into the well-known stationary solution to the problem, we also compare Δt with the corresponding exact analytical expression for the *phase delay time* $\tau_\theta = \hbar d\theta/dE$.

The paper is organized as follows. Section II presents the solution to the time-dependent Schrödinger equation for the δ potential barrier using cutoff plane waves as the initial condition. In Sec. III it is shown that the delay time follows from the interference transient terms. Finally, Sec. IV provides the concluding remarks.

II. TIME-DEPENDENT SOLUTION

We consider the solution of the time-dependent Schrödinger equation for tunneling through a δ barrier potential $V(x) = b\,\delta(x)$,

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + b\,\delta(x) \right) \Psi(x,t), \qquad (1)$$

with cutoff plane-wave initial conditions at $t=0$,

$$\Psi(x,k,t=0) = \begin{cases} e^{ikx}, & x<0 \\ 0, & x>0. \end{cases} \qquad (2)$$

The above initial condition may be visualized as a beam of particles of energy $E = \hbar^2 k^2/2m$, moving from the left, interrupted at $x=0_-$ by a perfectly absorbing shutter perpendicular to the beam [10]. At $t=0$, the shutter is opened and the transmitted probability density along $x>0$ as t evolves is

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investigated. To obtain the transmitted solution, we proceed along the same lines as in Ref. [11]. The Laplace transformed solution $\bar{\Psi}(x,s)$ reads

$$\bar{\Psi}(x,k,s) = \frac{im}{\hbar} \frac{e^{ipx}}{(p+i\beta)(p-k)}, \tag{3}$$

where $\beta = mb/\hbar^2$ and $p = \sqrt{2ims/\hbar}$. After a simple partial fraction decomposition, the inverse Laplace transform yields, for $x > 0$, the solution [12]

$$\Psi_\delta(x,k,t) = T(k)M(y_k) + R(k)M(y_{-i\beta}), \tag{4}$$

where $T(k)$ and $R(k)$ stand for the transmission and reflection amplitudes given, respectively, by

$$T(k) = \frac{k}{k+i\beta}, \tag{5}$$

and

$$R(k) = \frac{i\beta}{k+i\beta}. \tag{6}$$

The M's in Eq. (4) represent the functions $M(y_q)$, where q stands for k or $-i\beta$, that may be written in terms of the function w for complex argument [13],

$$w(iy_q) = e^{y_q^2} erfc(y_q), \tag{7}$$

as

$$M(y_q) = \frac{1}{2} e^{imx^2/2\hbar t} w(iy_q) \tag{8}$$

with the argument y_q defined as

$$y_q = e^{-i\pi/4} \left(\frac{m}{2\hbar t} \right)^{1/2} \left[x - \frac{\hbar q}{m} t \right]. \tag{9}$$

If the interaction vanishes, i.e., $b = 0$, the solution given by Eq. (4) goes into the free propagating solution [10],

$$\Psi_0(x,k,t) = M(y_k). \tag{10}$$

Note that the solution for $\Psi_\delta(x,k,t)$, given by Eq. (4), is formed by two terms. One of them is identical to the free solution multiplied by the transmission amplitude $T(k)$, whereas the other term is related to the purely imaginary pole at $k_a = -i\beta$ of the transmission (or reflection) amplitude of the problem, see Eqs. (5) and (6). We mention here that the general solution for an arbitrary potential also exhibits a free-type term and a contribution that is given as a sum over the complex poles of the corresponding transmission amplitude of the problem [8].

The long time behavior of the M functions follows immediately from the properties of the function $w(iy_q)$ [13]. Thus $M(y_k)$ goes as

$$M(y_k) \approx 2e^{y_k^2} + \frac{1}{\pi^{1/2} y_k} - \frac{1}{\pi^{1/2} y_k^3} + \cdots \tag{11}$$

and $M(y_{-i\beta})$ as

$$M(y_{-i\beta}) \approx \frac{1}{\pi^{1/2} y_{-i\beta}} - \frac{1}{\pi^{1/2} y_{-i\beta}^3} + \cdots. \tag{12}$$

At asymptotically long times, Eq. (11) goes into the exponential term $2\exp(y_k)^2$ and Eq. (12) tends to a vanishing value. Using Eq. (9) in Eq. (8), with $q = k$, one sees that the exact solution given by Eq. (4) becomes the stationary solution to the problem,

$$\Psi(x,k,t) = T(k) e^{ikx} e^{-iEt/\hbar}. \tag{13}$$

Clearly, at long times, the free solution $\Psi_0(x,k,t)$ behaves as Eq. (13) with $T = 1$.

Using Eq. (4), the corresponding probability density may be written as

$$|\Psi_\delta(x,k,t)|^2 = |\Psi_f(x,k,t)|^2 + |\Psi_\beta(x,k,t)|^2 + I(x,k;t), \tag{14}$$

where

$$\Psi_f(x,k,t) = T(k)M(y_k), \tag{15}$$

$$\Psi_\beta(x,k,t) = R(k)M(y_{-i\beta}), \tag{16}$$

and

$$I(x,k,t) = 2\,\mathrm{Re}[T(k)R^*(k)M(y_k)M^*(y_{-i\beta})] \tag{17}$$

stands for the interference contribution.

III. EXAMPLE

We proceed to analyze the time evolution of the probability density for both the δ potential barrier and the free case in order to characterize the delay time. We use parameters typical of semiconductor quantum structures [9], namely an effective mass for the electron $m = 0.067 m_e$, incidence energy $E = 0.08$ eV, and we choose the δ potential intensity $b = 0.427$ eV nm [14]. Figure 1 illustrates the behavior of the probability density for the δ and free cases (continuous and dashed lines, respectively) as a function of time for the fixed position $x_0 = 20$ nm. We can clearly appreciate the transient behavior in each curve and a shift of both wavefronts with respect to each other, which means that the particle that interacts with the potential takes a longer time to reach the position $x_0 = 20$ nm with respect to that evolving freely. A similar behavior has been reported in Ref. [12]. It is also worth noticing that the tunneling or transmitted probability density maintains a similar shape to that in the free case. This is due to the quasimonochromatic nature of the incidence initial state, which implies that there are not enough available k-space components to produce a transmitted wave packet suffering a noticeable deformation.

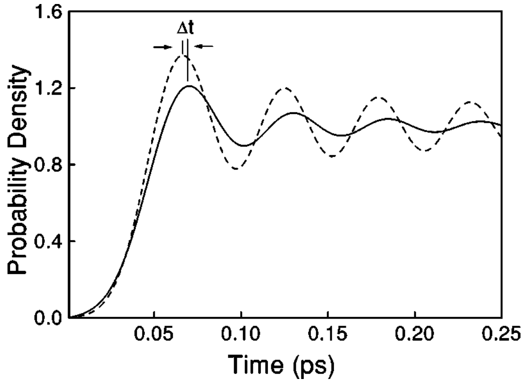

FIG. 1. Plot of $|\Psi_\delta(x_0,k,t)|^2$ (solid line) and $|\Psi_f(x_0,k,t)|^2$ (dashed line) as a function of the time t for a fixed value of the position $x_0=20$ nm. A delay time $\Delta t=3.8\times10^{-3}$ ps is appreciated. See text.

Measuring the time difference of the maximum values of $|\Psi_\delta(x_0,k,t)|^2$ (solid line) and $|\Psi_f(x_0,k,t)|^2$ (dashed line) given, respectively, by $t_{m\delta}$ and t_{mf}, allows us to calculate the *dynamical delay time*,

$$\Delta t=t_{m\delta}-t_{mf}, \tag{18}$$

as indicated also in Fig. 1. Repeating this procedure for increasing values of $x=x_0$ yields different values of Δt.

In Fig. 2 we plot Δt as a function of the position x_0 (circles). The dynamical character of Δt is clearly evident. One sees that as the position increases, Δt tends to a constant value that corresponds precisely to the *phase delay time* (dashed line) given by the exact analytic expression [15],

$$\tau_\theta=\frac{bm^2}{\hbar^3k[k^2+(mb/\hbar^2)^2]}. \tag{19}$$

If the interference term in Eq. (14) is eliminated, the delay time does not appear. This is shown in Fig. 3, which illustrates the behavior of the curves $|\Psi_\delta(x_0,k,t)|^2-I(x_0,k,t)$ (solid line) and $|\Psi_f(x_0,k,t)|^2$ (dashed line) at the fixed po-

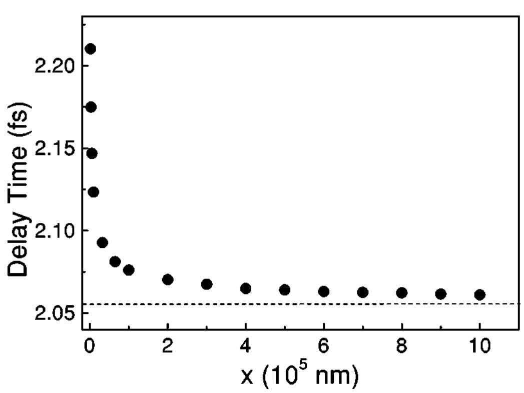

FIG. 2. This graph shows the delay time as a function of the position x. The circles indicate the numerical results obtained using Eq. (18) and the dashed line shows the phase time calculated using the analytic expression given by Eq. (19). The parameters are given in the text.

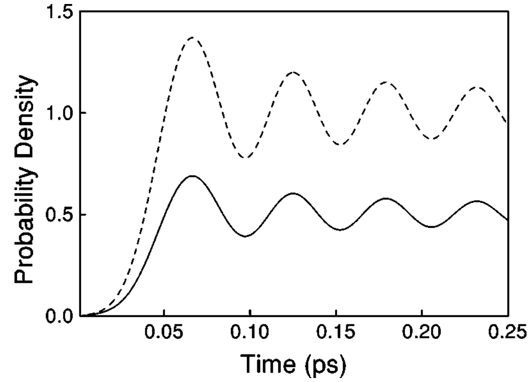

FIG. 3. Plot of the transmitted probability density without the interference term (solid line) and the free probability density (dashed line) to illustrate that the delay time occurs due to the interference term $I(x_0,k,t)$. See text.

sition $x_0=20$ nm as a function of time. The maxima of both curves occur at the same time. Therefore, the contribution of the interference term to the probability density $|\Psi_\delta(x_0,k,t)|^2$ is the one responsible for the delay time.

It is also of interest to investigate the delay time as a function of the intensity b of the δ potential for a fixed value of $k=k_0$. Figure 4 provides an example of such a calculation. One sees that there is a value of b where the *phase delay time* τ_θ (continuous line) exhibits a maximum. The above value occurs at $b=\hbar^2k_0/m$. This is interesting because it suggests a connection between the antibound pole of the transmission amplitude, Eq. (5), at $k_a=-ik_0$ and maximum delay time. Figure 4 also exhibits a comparison of the above exact calculation with the *dynamical delay time* Δt for different values of the distance x, 10^2 nm (black squares), 10^3 nm (black triangles), and 10^7 nm (black dots). One sees that as the distance increases, Δt tends to τ_θ, as expected.

IV. CONCLUDING REMARKS

The main result of this work is that the interference between the transient terms appearing in the exact analytical

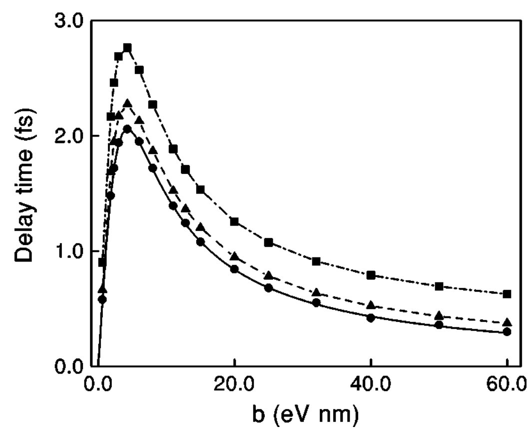

FIG. 4. Plot of τ_θ (continuous line) as a function of the intensity b of the δ potential, for a fixed value of k_0, to show that there is a maximum delay time at $b=\hbar^2k_0/m$ and also to compare it with Δt evaluated at different distances: $x=10^2$ nm (black squares), $x=10^3$ nm (black triangles) and $x=10^7$ nm (black dots). See text.

solution to the time-dependent Schrödinger equation for tunneling through a δ potential accounts for the delay time with respect to the corresponding free solution. This result provides insight into the dynamical processes involving a time-dependent description for tunneling using cutoff initial plane waves. We have also obtained that the *dynamical delay time* Δt given by Eq. (18) tends at asymptotically long times to the *phase time* τ_θ given by Eq. (19). However, at short distances and times, Δt increases and departs from the value given by the *phase time*. This result might be of interest in connection with the tunneling time problem because it tells us that *phase delay delay time* may not be an appropriate time scale near the interaction region. As a final remark, it is worth emphasizing the role played by the antibound pole of the transmission amplitude, $k_a = -imb/\hbar^2$, on the dynamics of the delay time. The exact analytic solution for more general potentials involves a summation over complex poles of the transmission amplitude [8,16,17], and one should expect, using arguments similar to those discussed here, that the corresponding transient interference terms will also be responsible for the delay time in these cases.

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[15] Writing the transmission amplitude as $T = |T| \exp(i\theta)$ allows us to write the phase time as $\tau_\theta = \hbar\, \mathrm{Im}[(dk/dE)(dT/dk)/T]$. Using Eq. (5) in the above equation leads to Eq. (19).

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