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Bound-state-induced persistent oscillations in the transient behavior of the probability density for the attractive δ potential

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An exact analytical solution to the time-dependent Schrödinger equation for an attractive δ potential using cutoff plane-wave initial conditions is derived to investigate the effect of a bound state on the transmission transients. We find that at short distances from the potential the probability density behaves harmonically at all times. This unexpected behavior, which corresponds to the trapping of a fraction of the transmitted wave, decreases exponentially with distance, so that at large distances the solution goes into the stationary solution. We find also that this behavior has no effect on the *phase time*.

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I. INTRODUCTION

Quantum transients are phenomena that vanish after a quantum system has reached the stationary regime [1]. One of the most representative examples is the *diffraction in time* phenomenon discussed by Moshinsky [2], in which a cutoff plane wave is confined initially to a semiplane in space by a perfectly absorbing shutter and then allowed to evolve freely. The quantum shutter setup can be generalized by placing in front of the shutter a one-dimensional finite range potential. An analytical solution for this problem was found by García-Calderón and Rubio [3] using the formalism of resonant states. The solution involves an expansion over the complex poles of the potential and the residues of the outgoing Green function of the problem.

A particular example considered before in the literature [4,5] comes from considering a repulsive δ potential. It is known that the solution comprises a quasimonochromatic term and a resonant term and this solution is known to hold for δ barriers and wells [6]. This potential is amenable for an analytical treatment and reflects the essential behavior of more realistic potentials.

In this paper we present a derivation of the solution for the attractive δ-potential case using the Laplace transform technique to investigate its transmission transients. We also study the effect of these transients on the *phase time*.

The simplicity of the solution that will be derived is related to the fact that the δ potential has only one complex pole. In more complex potentials there exist an infinite and discrete number of poles that follow certain trajectories on the complex p plane as a function of the potential parameters, but in the present case there is only one pole placed along the imaginary p axis; nevertheless, the difference in the pole location (above or below the origin) creates a very important distinction between positive and negative potentials in the behavior of the transients at short distances from the potential.

The bound-state trapping phenomenon was found in the context of a sudden change in a potential configuration of a decay problem, in which a well is shifted downward in energy [7]. Since its discovery, trapping has been associated with a perpetual interference between states in a certain region; however, it was found as a rather weak phenomenon. In this paper, trapping is the dominant phenomenon, and is free from the effect of any other transients.

This paper is organized as follows. Section II presents the derivation of the solution to the time-dependent Schrödinger equation for an attractive δ potential. In Sec. III a discussion of the transients found at short distances from the potential is given. Section IV shows that in the attractive δ-potential case there is a time advance with respect to the free-case solution at large distances. Section V presents the conclusions.

II. TIME-DEPENDENT SOLUTION

We solve the time-dependent Schrödinger equation for the attractive potential $V(x) = -b\delta(x)$, with $b > 0$,

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

with the initial condition

$$\Psi(x,0) = e^{ikx}\Theta(-x), \tag{2}$$

where $\Theta(x)$ refers to the Heaviside step function. Equation (2) corresponds to the quantum shutter initial condition, considered by Moshinsky for the free case [2]. The initial condition (2) may be visualized as a quasimonochromatic beam of particles of energy $E = \hbar^2k^2/2m$, moving from the left, and interrupted at $x = 0_-$ as previously mentioned. At $t = 0$ the shutter is opened and we may investigate the probability density along the transmitted region at a fixed distance $x = x_0$ as a function of time.

Laplace transforming Eq. (1) gives, along the transmission region, a solution that may be written as

$$\widetilde{\Psi}(x,p) = \frac{im}{\hbar}\left(t(k)\frac{e^{ipx}}{p(p-k)} + r(k)\frac{e^{ipx}}{p(p-i\beta)}\right), \tag{3}$$

where we have used the change of variable $p = \sqrt{2ims/\hbar})$, $\beta = mb/\hbar^2$, and

$$t(k) = \frac{k}{k-i\beta}, \quad r(k) = -\frac{i\beta}{k-i\beta} \tag{4}$$

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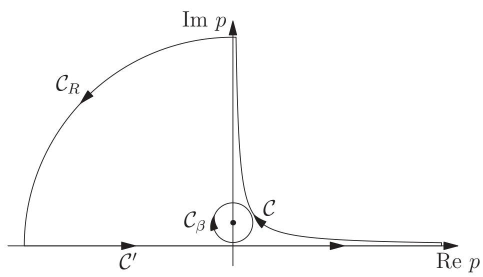

FIG. 1. Contour $\mathcal{C}$ for evaluating the solution in the δ-potential attractive case.

are, respectively, the transmission and reflection amplitudes of the time-independent problem. Using the theorem on the inverse Laplace transform [8] we may write

$$\Psi(x,t) = -\frac{\hbar}{2\pi m}\int_{\mathcal{C}} \widetilde{\Psi}(x,p)e^{-i\hbar p^2/2mt}\,p\,dp, \quad (5)$$

where $\mathcal{C}$ is the path depicted in Fig. 1. By substituting Eq. (3) into Eq. (5) and deforming the contour $\mathcal{C}$ as shown in Fig. 1, one sees that as the radius R of the semicircle goes to infinity, the factor $\exp(-i\hbar p^2 t/2m)$ in the integrand decreases rapidly and guarantees that the contribution from $\mathcal{C}_R$ vanishes exactly. Hence, one is left with the contribution coming from the residue at the bound pole $p = i\beta$ plus integral contributions along the real p axis. As a consequence, the solution $\Psi(x,t)$ may be written as

$$\Psi_\delta(x,t) = t(k)M(y_k) + r(k)M(y_{i\beta}), \quad (6)$$

where the Moshinsky function $M(y_k)$ is defined, for both real k and Im $k < 0$, as [9]

$$M(y_k) = \frac{i}{2\pi}\int_{-\infty}^{\infty}\frac{e^{ipx}e^{-i\hbar p^2 t/2m}}{p-k}dp = \frac{1}{2}e^{imx^2/2\hbar t}w(iy_k), \quad (7)$$

the function $w(z) = \exp(-z^2)\mathrm{erfc}(-iz)$ stands for the Faddeyeva function [10], and we have defined the Moshinsky function $M(y_{i\beta})$ for bound states (i.e., Im $i\beta > 0$) as

$$M(y_{i\beta}) = \tfrac{1}{2}e^{imx^2/2\hbar t}w(iy_{i\beta}) = e^{-\beta x}e^{i\hbar\beta^2/2mt} - \tfrac{1}{2}e^{imx^2/2\hbar t}w(-iy_{i\beta}). \quad (8)$$

The argument y_q, with $q = k, i\beta$ in Eqs. (7) and (8) is given by

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

Notice that the bound-state contribution in Eq. (6) results because the initial state is quasimonochromatic and hence it is not orthogonal to the bound state.

In the absence of the potential interaction (i.e., $b = 0$), Eq. (6) reduces to the free-case solution derived by Moshinsky [1,2]

$$\Psi_f(x,t) = M(y_k), \quad (10)$$

which at asymptotically long times goes into the stationary solution, namely, $\Psi_f \to \exp(ikx)\exp(-i\hbar k^2 t/2m)$ [2].

By using Eq. (6), we may write the probability density as

$$|\Psi_\delta(x,t)|^2 = |t(k)M(y_k)|^2 + |r(k)M(y_{i\beta})|^2 + 2\,\mathrm{Re}[t(k)r^*(k)M(y_k)M^*(y_{i\beta})]. \quad (11)$$

III. QUANTUM TRANSIENTS

Here we study the behavior of $|\Psi_\delta(x,t)|^2$ given by Eq. (11) as a function of time for distinct values of x in the transmission region. As an example we study the system with parameters $b = 0.427$ eV nm, $E = 0.08$ eV, and $m = 0.067m_e$ (m_e is the electron mass), which are the attractive case counterparts of the parameters considered in [4]. In Fig. 2 it is seen that at $x = 0_+$, $|\Psi_\delta(0_+,t)|^2$ exhibits at long times an oscillating behavior characterized by a definite amplitude A and period P. In order to analytically understand this behavior we notice that the condition of long times implies large values of the argument (9), and hence one may use asymptotic expansions for $w(iy_q)$ [10] to express the M functions in (6) for $x = 0$ as

$$M(y_q) \approx e^{-i\hbar q^2 t/2m} + \frac{1}{2\sqrt{\pi}\,y_q} - \frac{1}{4\sqrt{\pi}\,y_q^3} + \cdots, \quad (12)$$

where $q = k, i\beta$. It follows then by truncating the solution (6) in the leading exponential terms

$$\Psi_\delta(0,t) \approx t(k)e^{-i\hbar k^2 t/2m} + r(k)e^{i\hbar\beta^2 t/2m}. \quad (13)$$

The corresponding probability density at long times turns out to be

$$|\Psi_\delta(0,t)|^2 \approx 1 + \frac{2\beta k}{k^2+\beta^2}\sin\left(\frac{\hbar}{2m}(k^2+\beta^2)t\right), \quad (14)$$

which exhibits analytically a harmonic behavior of $|\Psi_\delta(0,t)|^2$ with time with an amplitude given by $A = 2\beta k/(k^2+\beta^2)$ and a period by $P = 4\pi m/\hbar(k^2+\beta^2)$ [11].

As is illustrated in Fig. 3, as x increases the oscillating behavior disappears. This can be shown analytically by

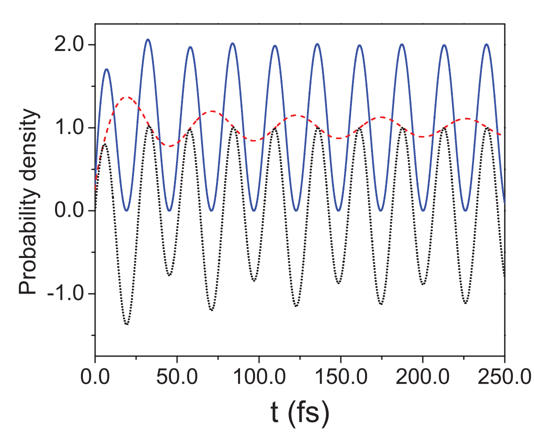

FIG. 2. (Color online) Comparison of the $|\Psi_\delta|^2$ (solid line), free-case solution $|\Psi_f|^2$ (dashed line), and $I(x,k,i\beta,t)$ (dotted line) contributions to the probability density for the δ potential plotted at $x = 0^+$ nm as a function of time with the parameters described in Sec. III.

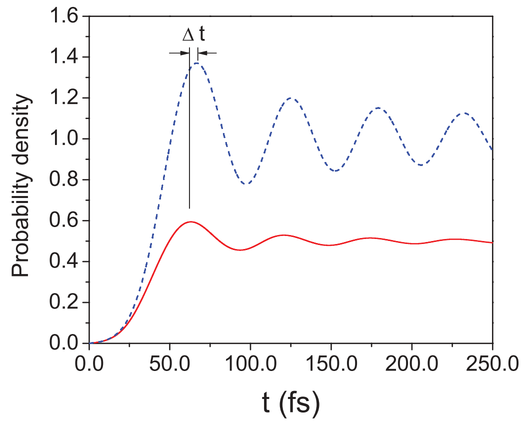

FIG. 3. (Color online) Plots of $|\Psi_\delta|^2$ (solid line) and $|\Psi_f|^2$ (dashed line) for the δ potential at $x = 20$ nm. It is seen that at large distances the probability density of the δ solution presents the transients observed in the diffraction in time phenomenon, but with a time advance with respect to the free-case solution. The parameters are the same as in Fig. 2. See text.

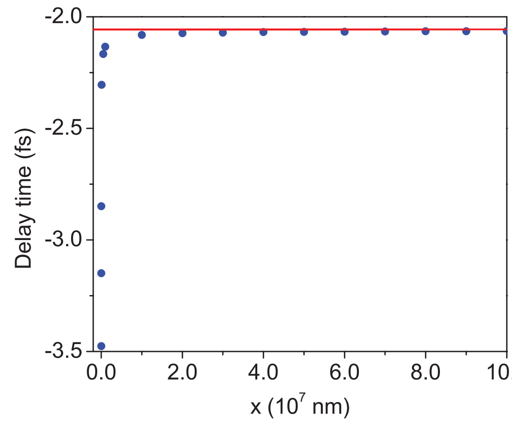

FIG. 4. (Color online) Plot of the dynamical delay time (full squares) and the phase delay time (solid line) as a function of the distance x from the potential for the attractive δ potential. The parameters are the same as in Fig. 2, for which $\tau_\theta = -2.05$ fs.

following a similar procedure as before with $x \neq 0$. In this case the solution to the leading exponential order is given by

$$\Psi_\delta(x,t) \approx t(k)e^{ikx}e^{-i\hbar k^2 t/2m} + r(k)e^{-\beta x}e^{i\hbar\beta^2 t/2m}. \quad (15)$$

The corresponding probability density may be written as $|\Psi(x,t)|^2 = T(k) + R(k)e^{-2\beta x} + I(x,k,i\beta,t)$, where $T(k) = |t(k)|^2$ and $R(k) = |r(k)|^2$ stand, respectively, for the transmission and reflection coefficients and the interference term $I(x,k,i\beta,t)$ reads

$$I(x,k,i\beta,t) = \frac{2\beta k}{k^2+\beta^2}e^{-\beta x}\sin\left(\frac{\hbar}{2m}(k^2+\beta^2)t - kx\right). \quad (16)$$

Notice that as x becomes very large, the oscillating contribution of Eq. (16) vanishes exponentially and we obtain $|\Psi(x,t)|^2 \to T(k)$.

IV. PHASE TIME

We find it interesting to explore the possible effect of the bound-state transient behavior on the the *phase delay time*. In our case, however, the attractive potential produces an *advance* or *negative delay time* of the solution with respect to the free case [12,13]. Here, we shall refer to this quantity as *phase advance time*. We study, in analogy to a similar investigation for the repulsive δ-potential case, an analysis of this time [4].

In a dynamical analysis, the phase time is obtained as the time difference between the maxima of the peaks of the transmitted and free evolving probability densities [4,14],

$$\Delta t = t_{m\delta} - t_{mf}, \quad (17)$$

where $t_{m\delta}$ and t_{mf} denote the times at which $|\Psi_\delta(x,t)|^2$ and $|\Psi_f(x,t)|^2$ attain, respectively, their first maximum value, as shown in Fig. 3. On the other hand, the phase time τ_θ, is defined as [15] $\tau_\theta = \hbar d\theta/dE = \hbar\, \mathrm{Im}[(dk/dE)(dt/dk)/t]$, where θ is the phase of the transmission amplitude [i.e., $t = |t|\exp(i\theta)$]. Inserting (4) into the above definition yields the exact analytical expression

$$\tau_\theta = -\frac{bm^2}{\hbar^3 k(k^2+\beta^2)}, \quad (18)$$

where the minus sign follows because the δ potential is attractive and hence yields a time advance.

Figure 4 exhibits a plot of Δt as a function of x for distances where the persistent oscillation is already negligible. For comparison, τ_θ is also plotted. One sees that at very large distances Δt tends to τ_θ.

As discussed in detail in Ref. [4] for the repulsive case, at large distances and times, the interference of $t(k)\exp(ikx)\exp(-iEt/\hbar)$ with the inverse power terms in the expansion of $M(-y_k)$ and $M(-y_{-i\beta})$ is responsible for the phase delay time. Notice that in our case, asymptotically $r(k)\exp(-\beta x)\exp(i\hbar\beta^2 t/2m)$ is negligible, and hence the same analysis as in Ref. [4] holds by changing the sign of β in the corresponding M function.

V. CONCLUSIONS

The δ potential possesses the advantage that it has only one simple pole, which in the attractive case considered here represents a bound state. It has been found that the bound-state pole of an attractive potential in the quantum-shutter setup induces, at short distances from the potential, a periodic oscillation in the probability density in the transmission region, an effect which is not damped in time but in distance. The source of this phenomenon is the interference between the quasimonochromatic and resonant pole contributions of the solution; this phenomenon is interpreted as a trapping of the initially confined wave.

Although the difference between attractive and repulsive δ potentials lies in the sign of its strength and hence in the character of the complex pole (bound or antibound), δ-potential transients for a repulsive potential behave very differently than those of their attractive counterparts. The transients for the repulsive potential exhibit damped oscillations in the transmission coefficient [4]; it is at long enough distances that both types of transients become similar, the only difference between them being an advance or delay time with respect to the free-case solution.

There is no reason to expect that the phenomenon of persistent oscillations discussed here is not present in other attractive potentials. For example, it occurs for square-well potentials, as will be discussed elsewhere. In spite of the fact that the quantum shutter setup refers to an idealized situation, it was able to predict the transient phenomenon of *diffraction in time* [2], which has been verified experimentally in recent years [1]. We hope that our finding of persistent oscillations in the probability density owing to the interference of bound-continuum states may also be the subject of experimental verification.

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