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Low-energy relativistic effects and nonlocality in time-dependent tunneling

Gastón García-Calderón
Instituto de Física, Universidad Nacional Autónoma de México, Apartado Postal 20-364, 01000 México, Distrito Federal, Mexico

Alberto Rubio*
Facultad de Ciencias, Universidad Autónoma de Baja California, Apartado Postal 1880, 22800 Ensenada, Baja California, Mexico

Jorge Villavicencio†
Centro de Investigación Científica y de Educación Superior de Ensenada, Apartado Postal 2732, 22800 Ensenada, Baja California, Mexico

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We consider exact time-dependent analytic solutions to the Schrödinger equation for tunneling in one dimension with cutoff wave initial conditions at $t=0$. We obtain that as soon as $t\neq 0$ the transmitted probability density at any arbitrary distance rises instantaneously with time in a linear manner. Using a simple model we find that the above nonlocal effect of the time-dependent solution is suppressed by consideration of low-energy relativistic effects. Hence at a distance x_0 from the potential the probability density rises after a time $t_0=x_0/c$ restoring Einstein causality. This implies that the tunneling time of a particle can never be zero. [S1050-2947(99)08903-9]

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Recent technological achievements such as the possibility of constructing artificial quantum structures at nanometric scales [1] or manipulating individual atoms [2] have stimulated a great deal of work at both the applied and fundamental level. In particular, studies on tunneling have addressed, among other things, the controversial question of the traversal time of a particle through a classically forbidden region [3]. The above considerations have motivated renewed attention regarding the time-dependent treatments of quantum tunneling. From the theoretical side, most of these works are based on the numerical analysis of the time-dependent Schrödinger equation with the initial condition of a Gaussian wave packet [4]. A common feature in most of these approaches is that the initial wave packet extends through all space. As a consequence the initial state, although it is manipulated to reduce as much as possible its value along the tunneling and transmitted regions, contaminates from the beginning the tunneling process. In the literature, however, one also finds a number of approaches to time-dependent tunneling, pionnered by Stevens [5], that in fact circumvent the above situation using a cutoff wave as initial state [5–8].

Our approach is a generalization to an arbitrary potential [8] of the Moshinsky shutter [9]. Moshinsky considered the solution of the time-dependent free Schrödinger equation with the initial condition, at $t=0$, of a plane wave of momentum k confined in the half-space region $x<0$ to the left of a perfectly absorbing shutter located at $x=0$. The sudden opening of the shutter at time $t=0$, allows the plane wave solution to propagate freely along the region $x>0$ [10]. Moshinsky showed that as the time t goes to infinity, the solution to the problem tends to the stationary solution. He also found that both the current and the probability density for a fixed value of the distance x_0 as a function of t, present oscillations near the wave front, situated at $t_0=x_0/v$. He named this phenomenon diffraction in time, in analogy to the well known phenomenon of optical diffraction. Recently an observation of diffraction in time has been reported [11]. If we put a potential barrier in the region $0\leqslant x\leqslant L$ with the same initial condition as above, then we may have a convenient model to analyze tunneling times by measuring at what time the probability density rises from zero. However, as pointed out by Holland [12] for the free case, and by García-Calderón and Rubio [8] for the case of a potential, the solution of the time-dependent Schrödinger equation for a cutoff initial plane wave has a nonlocal character. This means that if initially there is a zero probability for the particle to be at $x>0$, as soon as $t\neq 0$, there is instantaneously a finite, though very small, probability of finding it at any point $x>0$. This implies a zero tunneling time for some particles.

In this work we address the issue of the behavior of the time-dependent solution to the Schrödinger equation for tunneling through a potential barrier using a cutoff wave as initial condition. Our aim is to analyze the nonlocal behavior of the time-dependent transmitted solution at early times. We also study low-energy relativistic effects by solving the Klein-Gordon equation for a model potential. The implication of our findings for the tunneling time problem is briefly discussed.

*Deceased.

†Also at Facultad de Ciencias, Universidad Autónoma de Baja California Apartado Postal 1880, Ensenada, Baja California, Mexico.

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For the sake of simplicity in our approach we consider the instantaneous removal of the shutter. This may be seen as a kind of ''sudden approximation'' to a shutter opening with finite velocity, where the treatment is more involved even for the free case [13]. In a recent paper we have shown that the transmitted solution for the Schrödinger case for tunneling through an arbitrary potential barrier may be written as a free term solution plus an infinite sum of resonance transient terms associated with the S-matrix poles of the problem [8]. This corresponds to solve the time-dependent Schrödinger equation for a potential $V(x)$ that vanishes outside the region $0 \leqslant x \leqslant L$, with the initial condition,

$$\psi_s(x,k,t=0) = \begin{cases} e^{ikx}, & x<0, \\ 0, & x>0. \end{cases} \tag{1}$$

The transmitted solution for the region $x \geqslant L$ reads [8]

$$\psi_s(x,k,t) = T(k)M(x,k,t) - i\sum_n^{\infty} T_n M(x,k_n,t), \tag{2}$$

where $T(k)$ stands for the transmission amplitude of the problem, $T_n = u_n(0)u_n(L)\exp(-ik_nL)/(k-k_n)$, is given in terms of the resonant eigenfunctions $u_n(x)$ and complex S-matrix poles k_n; and the Moshinsky functions $M(x,k,t)$ and $M(x,k_n,t)$ are defined as

$$M(x,q,t) = \tfrac{1}{2} e^{(imx^2/2\hbar t)} e^{y^2} \operatorname{erfc}(y), \tag{3}$$

where and the argument y is given by

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

In the above two equations q stands either for k or k_n. In the absence of a potential the solution given by Eq. (2) becomes the solution for the free case obtained by Moshinsky [9],

$$\psi_s^0(x,k,t) = M(x,k,t). \tag{5}$$

As discussed by Moshinsky, the initial condition given by Eq. (1) refers to a shutter that acts as a perfect absorber (no reflected wave). One can also envisage a shutter that acts as a perfect reflector. In such a case the initial wave may be written as

$$\psi_s(x,k,t=0) = \begin{cases} e^{ikx} - e^{-ikx}, & x<0, \\ 0, & x>0. \end{cases} \tag{6}$$

The transmitted solution for the region $x \geqslant L$ now reads

$$\psi_s(x,k,t) = T(k)M(x,k,t) - T(-k)M(x,-k,t) - 2ik\sum_n^{\infty} T_n M(x,k_n,t), \tag{7}$$

where $T_n = u_n(0)u_n(L)\exp(-ik_nL)/(k^2-k_n^2)$. The solution for the free case with the reflecting initial condition is

$$\psi_s^0(x,k,t) = M(x,k,t) - M(x,-k,t). \tag{8}$$

The exact solutions given by Eqs. (2) and (7), corresponding, respectively, to absorbing and reflecting initial cutoff waves, involve each a contribution proportional to the free case solution and then an infinite sum involving the S-matrix poles, $\{k_n\}$, and resonant states, $\{u_n(x)\}$, of the system. As shown in Ref. [8], at very long times, the terms $M(x,k_n,t)$ that appear in the above equations vanish. The same occurs for $M(x,-k,t)$ while, as shown first, to our knowledge, in Ref. [9], $M(x,k,t)$ tends to the stationary solution. Hence, at long times, each of the above exact solutions go into the stationary solution $T(k)\exp[i(kx-Et/\hbar)]$.

At very short times, for a given $x \geqslant L$, the argument of $M(x,k,t)$, given by Eq. (4) with $q=k$, becomes very large and in fact becomes independent of the value of k, $y \approx \exp(-i\pi/4)[m/2\hbar t]^{1/2}x$. Since for very large y, $M(y) \sim 1/y$ [9,8], it follows that $M(x,k,t)$ goes like $t^{1/2}$. As discussed also in Ref. [8], the functions dependent on the poles, $M(x,k_n,t)$, behave in a similar fashion provided the value of $t=t_0$ is sufficiently small to guarantee, for a fixed $x=L$, that $L \gg \hbar|k_n|t/m$. Since the distribution of the complex S-matrix poles on the k plane fulfills $[|k_1|<|k_2|\cdots<|k_n|\cdots$, one sees that as t becomes smaller and smaller there will be more and more values of n for which the corresponding M functions goes like $t^{1/2}$ as do all the rest of M functions associated with smaller values of n. In the appropriate limit as $t \to 0$ and $n \to \infty$, the corresponding M function then vanishes as $t^{1/2}$. Consequently for $x \geqslant L$, the solutions given by Eqs. (2) and (7) are proportional to $t^{1/2}$, namely,

$$\psi_s(x,k,t) \sim \frac{A}{x} t^{1/2} \quad (x \geqslant L), \tag{9}$$

where A is a constant. Note that at $t=0$ the solution vanishes in accordance with the initial condition. It is not difficult to see that Eq. (9) will hold also for a cutoff initial condition that is something between the initial conditions considered above, and more generally, for a wave packet formed by a linear combination of cutoff waves. Equation (9) tells us that the probability density at any distance x from the potential will rise instantaneously with time. This intriguing nonlocal behavior implies that an ideal detector will measure a zero tunneling time. The existence of action-at-a-distance effects in the time-dependent Schrödinger equation should not, in principle, pose any conceptual difficulties since the treatment is nonrelativistic. However, one could ask whether the above nonlocal behavior arises because the initial condition is a cutoff wave. In order to answer the above question we consider low-energy relativistic effects by solving the Klein-Gordon equation with a cutoff wave as initial condition for a simple potential model. Moshinsky [9] solved the Klein-Gordon equation for the free shutter problem with the initial condition of a cutoff plane wave in the region $x<0$ and showed that the probability density at a point $x>0$ is nonzero only after a time $t_0 > x_0/c$, with c the velocity of light. To our knowledge, a numerical analysis of this solution has not yet been performed. We would like to learn also how the relativistic solution is affected at early times by tunneling through a potential.

A potential that has been widely used in studies on time-dependent tunneling is the square barrier, characterized by a height V_0 and a width L. This potential has an infinite set of

S-matrix poles situated at increasing energies on top of the barrier. There is, however, a simpler potential model that is more amenable for a relativistic treatment. This is the δ potential $V(x)=b_s\delta(x)$. The solution corresponding to the time-dependent Schrödinger equation has been obtained by Elberfeld and Kleber using a δ-function propagator [14]. One can also follow a derivation by Laplace transforming directly the time-dependent Schrödinger equation of the problem using the initial condition given by Eq. (1) [15]. Defining $p^2=2ims/\hbar$ the Laplace transformed solution $\overline{\psi}_s(x,s)$ for the region $x>0$ reads

$$\overline{\psi}_s(x,k,s)=\frac{im}{\hbar}\frac{e^{ipx}}{(p+ib)(p-k)}, \tag{10}$$

where $b=mb_s/\hbar^2$. After a simple partial fraction decomposition the inverse Laplace transform yields, for $x>0$,

$$\psi_s^\delta(x,k,t)=T(k)M(x,k,t)+R(k)M(x,-ib;t), \tag{11}$$

where $T(k)$ and $R(k)$ stand for the transmission and reflection amplitudes for the stationary situation, $T(k)=k/(k+ib)$ and $R(k)=ib/(k+ib)$. Note that here instead of an infinite number of S-matrix poles the only S-matrix pole corresponds to an antibound state located at $k_a=-ib$. At a very short time one can easily see that $\psi_s^\delta(x,k,t)$ goes like $t^{1/2}$ fulfilling also, as the square barrier, Eq. (9).

The shutter problem for the Klein-Gordon equation with the δ potential $V(x)=b_r\delta(x)$ requires the solution of

$$\frac{\partial^2}{\partial x^2}\psi_r^\delta(x,k_r,t)=\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi_r^\delta(x,k_r,t)+[b_r\delta(x)+\mu^2]\psi_r^\delta(x,k_r,t), \tag{12}$$

where $\mu=mc/\hbar$. with the initial condition given by

$$\psi_r^\delta(x,k_r,t=0)=\begin{cases} e^{ik_rx}, & x<0,\\ 0, & x>0,\end{cases} \tag{13}$$

where we define $E_r^2=k_r^2+\mu^2$ and $k_r=k(1-(k/\mu)^2)^{-1/2}$. Note that E_r is given in units of the reciprocal length, i.e., $E_r\equiv E/\hbar c$. The condition given by Eq. (13) follows from the fact that, for $t<0$, when the shutter was closed, we had on the left side of the shutter, $\psi^\delta(x,k_r,t)=\exp[i(k_rx-E_rct)]$, for $x<0$ and a vanishing value for $x>0$. By direct application of the Laplace transform method one gets a set of differential equations corresponding to the regions $x>0$ and $x<0$. In order to derive an expression for the transmitted wave function, we have to consider the matching conditions to take into account the discontinuity of the wave function derivatives at $x=0$, obtaining the Laplace-transformed solution,

$$\overline{\psi}_r(x,s)=\frac{1}{2}\frac{(s-icE_r)}{(q+b_0c)(q+ik_rc)}e^{-qx/c}. \tag{14}$$

where $q=[s^2+\mu^2c^2]^{1/2}$ and $b_0=b_r/2$. Using the Bromwich contour to evaluate the inverse Laplace transform of Eq. (14) it is convenient to make the change of variable [9] $-iu=(q+s)/(\mu c)$. In this form $q=i\mu c(u^{-1}-u)/2$ and as a consequence the branch points at $s=\pm i\mu c$ go into an essential singularity at $u=0$ and two simple poles located on the lower half of the complex u plane. After separating into partial fractions one then may evaluate the resulting integrals by standard complex variable techniques to obtain the wave function,

$$\psi_r^\delta(x,k_r,t)=\begin{cases} A\psi_r^0(x,k_r,t)+BC\psi_r^0(x,-ib_0,t)+BD[\psi_r^0(x,-ib_0,t)]^*, & t>x/c,\\ 0, & t<x/c,\end{cases} \tag{15}$$

where $A=k_r/(k_r+ib_0)$, $B=ib_0/(k_r+ib_0)$, $C=(\epsilon+E_r)/(2\epsilon)$, and $D=(\epsilon-E_r)/(2\epsilon)$, and also $\epsilon=(\mu^2-b_0^2)^{1/2}$. In Eq. (15), the function $\psi_r^0(x,k_r,t)$ is the solution of the free Klein-Gordon case [9,16], namely,

$$\psi_r^0(x,k_r,t)=\begin{cases} e^{i(k_rx-E_rct)}+\frac{1}{2}J_0(\eta)-\sum_{n=0}^{\infty}[\xi/iz]^nJ_n(\eta), & t>x/c,\\ 0, & t<x/c,\end{cases} \tag{16}$$

where $J_n(\eta)$ stands for the Bessel function of order n and,

$$\xi=\left[\frac{ct+x}{ct-x}\right]^{1/2},\quad \eta=\mu(c^2t^2-x^2)^{1/2},\quad z=\frac{1}{\mu}(k_r+E_r). \tag{17}$$

The expressions, $\psi_r^0(x,-ib_0,t)$ and $[\psi_r^0(x,-ib_0,t)]^*$ in Eq. (15) have the same form as the free solution in Eq. (16) with k_r replaced by $-ib_0$. Asymptotically for very long times in the solution $\psi_r^\delta(x,k_r,t)$, given by Eq. (15), the terms $\psi_r^0(x,-ib_0,t)$ and $[\psi_r^0(x,-ib_0,t)]^*$ vanish, while the term $\psi_r^0(x,k_r,t)$ goes into the stationary solution $\exp[i(k_rx-E_rct)]$.

To exemplify the above results Fig. 1 exhibits the very short time behavior of the probability density for the delta potential at a fixed distance $x=L=0.3$ Å. One sees that the Schrödinger description (broken line), obtained from Eq. (11) with parameters $b_s=2.0$ eV-Å and $E=0.01$ eV, yields an instantaneous response with time while the relativistic solution, calculated using Eq. (15), starts after t_0

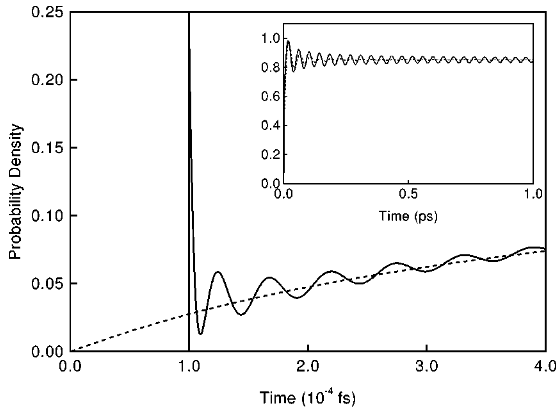

FIG. 1. Plot of $|\psi_s^\delta(x,t)|^2$ (dashed line) and $|\psi_r^\delta(x,t)|^2$ (solid line), respectively, for the Schrödinger and Klein-Gordon solutions for a δ potential, as a function of time at a fixed distance at early times and at long times (inset). See text.

$=L/c$. This tell us something relevant: The nonlocal behavior of the Schrödinger description is due to its nonrelativistic nature. The nonlocal behavior of the Schrödinger solution would result from the fact that in a nonrelativistic description there is no restriction on the velocity of some components of the initially confined wave function. The sharp relativistic wave front of height 0.25 in Fig. 1 follows as a consequence of the initial condition given by Eq. (13). This jump occurs also in the free case and may be obtained analytically [9]. For an initial function of the type

$$\exp(ik_r x)+\exp(i\alpha)\exp(-ik_r x), \quad (x<0),$$

with α an arbitrary phase, the peak height will be a function of α. In particular, for a reflecting initial condition, ($\alpha=\pi$), the solution starts smoothly from zero at $t_0=L/c$. It might be of interest to mention that in fully relativistic quantum field theories Hegerfeldt [17] has pointed out that the sudden opening of a shutter may lead to violation of Einstein causality, i.e., no propagation faster than light. This author has argued that the difficulty is of a theoretical nature and has discussed some ways to solve it. Our relativistic model satisfies Einstein causality. The inset to Fig. 1 shows that at longer times the above two solutions approach each other, both presenting the characteristic transient behavior near the "classical" wave front at $x=vt$, which in our example occurs at a very short time. Our analysis has a consequence of interest for the tunneling time problem. Since the probability density rises with time after a time $t_0=x_0/c$, it implies that the tunneling time of a particle can never be zero, contrary to some claims in the literature [3].

Thus we can see that a proper description of the quantum mechanical propagation for the transmitted solution, even at low energies, strictly requires a relativistic treatment. However, since the corresponding solutions are practically identical up to the relativistic cutoff, at $t=L/c$, suggests that the Schrödinger description is quite accurate provided the velocity components larger than c are omitted.

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