Effects of relativity on the time-resolved tunneling of electron wave packets

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We solve numerically the time-dependent Dirac equation for a quantum wave packet tunneling through a potential barrier. We analyze the spatial probability distribution of the transmitted wave packet in the context of the possibility of effectively superluminal peak and front velocities of the electron during tunneling. Both the Dirac and Schrödinger theories predict superluminal tunneling speeds. However, in contrast to the Dirac theory the Schrödinger equation allows a possible violation of causality. Based on an analysis of the tunneling process in full temporal and spatial resolution, we introduce an instantaneous tunneling speed that can be computed inside the potential barrier.

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I. INTRODUCTION

The phenomenon of tunneling in which a quantum-mechanical particle can penetrate a repulsive barrier with a height that exceeds the total energy of the particle is counterintuitive. Any explanation or intuition for this process based on classical mechanics fails. At the same time, this effect is extremely important and has been studied widely. The Josephson effect in high-speed semiconductors [1], β decay in nuclear physics, and instantons in high-energy physics are just a few examples. In the early 1930s it was already recognized that there was no appreciable temporal delay in the transmission of wave packets through barriers [2]. Wigner discussed the possibility that a particle can effectively travel faster than the speed of light when passing through the barrier. Chiao and co-workers have more recently addressed the realization of superluminal speeds in a more systematic way. They used a periodic potential barrier to demonstrate experimentally that superluminal velocities can indeed be obtained, and showed that this result does not violate causality.

In this article we intend to address the following questions: Can one trust the predictions of a nonrelativistic theory at all if superluminal effects are being investigated? How accurate are these predictions? Does the relativistic quantum theory predict superluminal speeds? Does a fully relativistic treatment of tunneling increase or reduce the tunneling probability? Does the existence of superluminal velocities imply the violation of Einstein's causality when they are computed in the framework of the Schrödinger equation? Can causality be restored in the Dirac theory? Can one define a physical quantity that describes the time evolution of a wave packet inside the barrier which reduces to the regular peak velocity when calculated from a wave packet that is outside the barrier? Due to its lacking a counterpart in classical mechanics, it is not obvious how to apply any intuition to relativistic quantum-mechanical tunneling and to predict any answers to these questions. A full Dirac theory calculation seems necessary.

Quite remarkably, despite the large amount of literature on nonrelativistic tunneling, we are aware of only two works [3] that have addressed some of these questions. Leavens and Aers [3] used the stationary-state approach to analyze Larmor-clock transmission times for single and double rectangular barriers. In some special cases the problem of quantum-mechanical tunneling can be mapped onto the fully relativistic problem of evanescent electromagnetic radiation [4–7].

For the special case of nonrelativistic tunneling, the question of how much time it takes a particle to pass the barrier has triggered considerable controversial debate to the present day. Even though by 1993 the community had largely accepted the fact that there actually is a time scale associated with the duration of tunneling, there is still a lack of consensus with regard to the existence of a unique expression for this time scale and on the exact implications of this expression [8]. In fact, Hauge and Stovneng [9] stated that with the exception of two candidates all expressions for tunneling times have logical flaws sufficiently serious that they must be rejected. The only two survivors are the dwell time [10] and the asymptotic phase time [8,9], which have complementary weaknesses.

In this article, we stay away from most of the controversial issues and focus on investigating the effect of relativity on the tunneling process. Our model system is an electron that tunnels through a one-dimensional repulsive barrier. The time evolution of this system is given by the solution of the Dirac equation

$$i\partial\Psi/\partial T = -ic\alpha_x\partial\Psi/\partial x + c^2\beta\Psi + W(x)\Psi, \qquad (1.1)$$

where the repulsive potential $W(x)$ is centered around $x=0$ and has an effective width of w and a height W_0. In order to check the generality of our results we have used a variety of different tunneling potentials $W(x)=W_0\exp[-(2x/w)^n]$. For large even integers n we recover the rectangular barrier for which the energy eigenstates can be found analytically and also some approximate analytical estimates can be derived. Here α_x and β denote the 4×4 Dirac matrices. The time-dependent solution of the spinor wave function $\Psi(x,T)=[\Psi_1,\Psi_2,\Psi_3,\Psi_4]$ can be obtained numerically on a space-time grid using a split-operator algorithm based on fast Fourier transformation that is accurate up to fifth order in time [11]. In all of our simulations, the spatial axis was discretized into at least 65 536 grid points which together with up to 1 500 000 temporal points led to fully converged results.

As an incoming electron wave packet we used the state

$$\Psi(x,T=0)=N\exp[-(x-x_0)^2/(4\Delta x^2)]\exp(ik_0x)\psi(k_0), \tag{1.2}$$

where the spinor $\psi(k_0)$ is given by $[1,0,0,ck_0/(E_0+2c^2)]$ and the normalization factor $N\equiv[(E_0+2c^2)/(2(E_0+c^2)\Delta x\sqrt{2\pi})]^{1/2}$. Here the total energy $E_0\equiv\sqrt{[c^4+c^2k_0{}^2]}-c^2$. The central canonical momentum k_0 is related to the initial speed v_0 via $v_0=k_0/\sqrt{[c^2+k_0{}^2]}$. We should mention that, instead of a Gaussian distribution in position space, we could have equally well chosen a Gaussian in momentum space, which in the nonrelativistic limit $v_0\ll c$ would yield the same state as Eq. (1.2). The initial location of the wave packet x_0 was chosen far enough to the left of the barrier that the total spatial probability for positive values of x was negligible at time $T=0$. The total energy $E_0=\sqrt{[c^4+c^2k_0{}^2]}-c^2$ in our case will be consistently chosen smaller than W_0. The potential height W_0 was also chosen smaller than $2c^2$ to avoid the effect of the negative-energy continuum as characteristic of the so-called Klein paradox [11–13]. This will restrict our initial velocities to $v_0<0.94c$ $(=129\text{ a.u.})$. The potential height W_0 was chosen to be 1.5 times the kinetic energy E_0 such that we can essentially exclude the effect of high-momentum contributions that can simply pass over the barrier without tunneling. Please note that the predictions of the corresponding Schrödinger equation can be obtained quite conveniently in our numerical simulations by increasing the ''parameter'' c to infinity [14].

The most direct way to ''measure'' the electron's speed inside the barrier would be to compare its ''position'' at various times during the tunneling. However, the wave functions are essentially delocalized during the scattering event and previous definitions of effective average tunneling velocities under the barrier were based on extrapolating the information from the positive or negative spatial delay of the scattered wave packets outside the tunneling region. After a discussion of these effective velocities and a critical analysis of their regime of validity, we will propose in the last section an instantaneous tunneling speed that can be calculated directly from the wave packet inside the barrier. It turns out that the dynamics can be roughly divided up into two regimes depending on the relative magnitude of the initial spatial width in the Gaussian wave packet Δx and the barrier width w. We will discuss them separately below.

II. THE RELATIVISTIC MODIFICATION OF THE WIGNER TUNNELING SPEED

A. Spatially broad wave packets: $\Delta x>w$

With the exception of an overall amplitude reduction the wave packet does not get significantly distorted as it tunnels through the barrier for the case $\Delta x>w$. In this regime the center of mass for the transmitted wave packet (denoted in the following by $\langle x\rangle_t$) agrees approximately with the peak value of the spatial probability density. For the nonrelativistic case this regime has been studied very intensively as the stationary-phase approximation is qualitatively reliable, permitting some analytical investigations based on the phase of the complex transmission amplitude. Below we will test this approximation and compare it with the exact numerical solution of the time-dependent Dirac and Schrödinger equations.

For the special case of $n\to\infty$ in the mentioned model potential we recover the rectangular barrier, for which the complex transmission amplitude can be derived fully analytically as $|t(k,w,W_0)|\exp[i\alpha(k,w,W_0)]$, where

$$t(k,w,W_0)=\frac{\exp[-ikw]}{\cosh(\kappa w)+i[(1-\Gamma^2)/2\Gamma]\sinh(\kappa w)}, \tag{2.1}$$

$$\alpha(k,w,W_0)=-kw-\tan^{-1}\left[\frac{(1-\Gamma^2)}{2\Gamma}\tanh(\kappa w)\right], \tag{2.2}$$

and where

$$\kappa\equiv\frac{1}{c}\sqrt{c^4-(E+c^2-W_0)^2}\quad\text{and}$$

$$\Gamma\equiv\sqrt{E(E+2c^2-W_0)/(E+2c^2)(W_0-E)}.$$

Comparing the tunneling probability $|t(k,w,W_0)|^2$ obtained from Eq. (2.1) with its nonrelativistic limit (calculated from setting $c\to\infty$) we find that relativity reduces the tunneling efficiency but increases the effective tunneling speed as we will see below; a result that might be counterintuitive.

In the stationary-phase approximation discussed below, the center of the transmitted wave packet $\langle x(T)\rangle_t$ at time T can be calculated from

$$\langle x(T)\rangle_t=x_0-\left.\frac{d\alpha(k)}{dk}\right|_{k_p}+\left.\frac{dE(k)}{dk}\right|_{k_p}T, \tag{2.3}$$

where the energy $E(k)\equiv\sqrt{[c^4+c^2k^2]}-c^2$, and the right-hand side has to be evaluated at the momentum k_p for which the product of the absolute value of the momentum amplitude and $|t|$ takes its maximum value. After some algebra we obtain

$$-\frac{d\alpha(k)}{dk}=w-\frac{c^2k}{2(E+c^2)[1+[(1-\Gamma^2)^2/4\Gamma^2]\tanh^2(\kappa w)]}\times\left\{\frac{W_0}{2}\left(\frac{1}{\Gamma}+\Gamma\right)\tanh(\kappa w)\left[\frac{1}{E(W_0-E)}+\frac{1}{(E-W_0+2c^2)(E+2c^2)}\right]+\frac{w}{\kappa}\left(\frac{1}{\Gamma}-\Gamma\right)\times\operatorname{sech}^2(\kappa w)\left[1-\frac{(W_0-E)}{c^2}\right]\right\}, \tag{2.4}$$

$$\frac{dE(k)}{dk}=\frac{c^2k}{\sqrt{c^4+c^2k^2}}. \tag{2.5}$$

Equation (2.4) predicts that the distance $-d\alpha(k)/dk|_{k_0}$ is always smaller than w; in other words, the tunneling process cannot advance the packet by more than the width of the potential. Only if the tunneling were to happen instantaneously could we obtain a spatial shift with its maximum value w. This is consistent with the condition of the validity of the stationary-phase approximation, which requires that the momentum scale on which the phase $\alpha(k)$ varies ($\approx \alpha/[d\alpha(k)/dk]$) should be larger than the momentum width of the Gaussian wave packet Δk.

The parameter $1/(2\Delta x)=\Delta k$ is the momentum width according to the Heisenberg uncertainty relation. If Δk is smaller than the momentum scale on which $t(k)$ varies, i.e., $\Delta k<|t|/[d|t(k)|/dk]$, then the central velocity of the transmitted wave packet, denoted by $v_t=\langle\Psi_t|c\alpha_x|\Psi_t\rangle$, agrees with that of the initial wave packet, $v_t\approx v_0$, such that the distance between the peaks of the transmitted packet and one that propagated without any barrier is just given by $\langle x(T)\rangle_t-\langle x^{(0)}(T)\rangle=-d\alpha(k)/dk|_{k_0}$, where $k_0=v_0/\sqrt{1-v_0^2/c^2}$.

The fact that the propagation velocities on the two sides of the barrier can be different ($v_t>v_0$) [15] has been noted earlier for the nonrelativistic case. Because $|t(k)|$ always increases monotonically with k, the smaller momentum components in the wave packet are attenuated more during the tunneling, such that the emerging ''truncated'' wave packet has higher average momentum. This effect has been described in the literature as an effective electron acceleration [8,16]. For the case where k_p is significantly larger than k_0, the distance $\langle x(T)\rangle_t-\langle x^{(0)}(T)\rangle$ between the peaks of the tunneled and (barrier) free-wave packet increases as a function of time. In order to provide a more unambiguous comparison, the tunneled wave packet could be compared with a special free-wave packet whose initial momentum amplitudes were multiplied initially by the transmission amplitude $|t(k)|$, in order to compensate for the attenuated low-momentum components and to have the same average velocity v_t as the tunneled packet. In this comparison, the distance between the peaks $\langle x(T)\rangle_t-\langle\tilde{x}^{(0)}(T)\rangle$ does not depend on time and is equal to

$$D\equiv\langle x(T)\rangle_t-\langle\tilde{x}^{(0)}(T)\rangle=-d\alpha(k)/dk|_{k_0}. \qquad (2.6)$$

Clearly, without any ambiguity, this parameter D can be calculated directly from the wave packet. To associate an *effective* average tunneling velocity across the potential with this distance D, we define a quantity v_e as

$$v_e\equiv\frac{w}{T-(T_1+T_2)} = \frac{w}{T+(w/2+x_0)/v_0+[w/2-\langle x(T)\rangle]/\langle v(T)\rangle_t}, \qquad (2.7)$$

where $T_1\equiv(-w/2-x_0)/v_0$ and $T_2\equiv[\langle x(T)\rangle_t-w/2]/\langle v(T)\rangle_t$ correspond to the time intervals spent outside the potential region $-w/2<x<w/2$. If $v_0=v_t$ this definition reduces to $v_e=v_0w/(w-D)$. At this point we should stress that the ''speed'' v_e is just a defined quantity similar to the concept of a ''tunneling time.'' It is by no means clear whether the propagation of the peak through the barrier is really a microscopically correct physical picture in describing the center-of-mass motion as it tunnels through the barrier. We will comment on this question in more detail in Sec. III. Here we plot the ''speed'' defined in Eq. (2.7) in Fig. 1 as function of the barrier width w. The graphs turns out to be quite helpful in many respects.

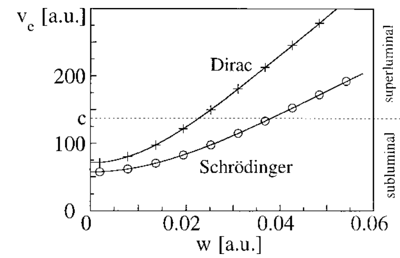

FIG. 1. Comparison of the relativistic and nonrelativistic predictions for the tunneling speed defined in Eq. (2.7). The solid lines are the predictions from the approximate analytical relativistic and nonrelativistic theories. The open circles and crosses are obtained from the exact spatial probability densities calculated from the Schrödinger and Dirac equations. The parameters were $x_0=-100$ a.u., $\Delta x=20$ a.u., $v_0=100$ a.u., $T=2$ a.u., and $W_0=1.5E_0$.

First of all, we should mention that the markers correspond to the exact wave-packet solutions to the time-dependent Schrödinger (circles) and Dirac (crosses) equations. For the Dirac case we have computed the quantum-mechanical spatial probability density $P(x,T)=\Sigma_{i=1}^4|\Psi_i(x,T)|^2$, where the summation extends over the four spinor components. For each barrier width w we have evolved the initial wave packet in time and then measured the distance D between the maxima of the tunneled and force-free wave packets which was then converted into the effective speed v_e according to Eq. (2.7). In each case the peak position differed by less than $10^{-2}\%$ from the center of mass of the packet. So the transmitted state is quite symmetric for these parameters. The agreement between the exact numerical data and the analytical prediction shows that the stationary-phase approximation leading to Eq. (2.3) is reliable in the relativistic and nonrelativistic cases for these parameters.

Second, having established the validity of the approximation in Eq. (2.3), we point out the difference between the relativistic and nonrelativistic tunneling speeds. For our initial velocity of $v_0=100$ a.u. the nonrelativistic tunneling speed v_e turns out to be 20% smaller than the relativistic speed. This result is a little surprising as one typically expects that smaller velocities are associated with relativistic corrections such as the nonlinear mass increase. In fact our result is in contrast to that of Leavens and Aers [3], who reported a reduction of the tunneling speed due to relativity for the case of a double-rectangular potential.

Relativistic as well as nonrelativistic theories consistently predict that for a sufficiently large barrier width ($w>0.023$ and 0.038 a.u., respectively) the effective tunneling speed can exceed the speed of light and become superluminal. In

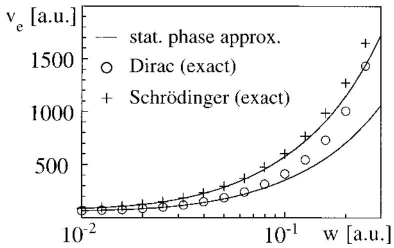

FIG. 2. The same graph as in Fig. 1 but on a larger scale of width w to show the breakdown of the analytical predictions for $w > \Delta x$. Same parameters as in Fig. 1, but $\Delta x = 4$ a.u..

fact, for a large barrier width w, the tunneling velocity v_e given in Eq. (2.7) simplifies because the spatial delay takes the form

$$D = w - \frac{c^2 k W_0 \Gamma}{(1+\Gamma^2)E(E+c^2)(W_0 - E)} \times \left[1 + \frac{E(W_0 - E)}{(E+2c^2)(E+2c^2-W_0)} \right]. \tag{2.8}$$

In the nonrelativistic case this phenomenon is called the Hartman effect [17], when $D(c \to \infty) = w - \sqrt{2/(W_0 - E)}$, and $v_e \to v_0 w \sqrt{(W_0 - E)/2}$ increases linearly with w.

Third, the two graphs for $w = 0$ are different from the initial velocity v_0 as one could have conjectured. In fact, the regime of small barrier widths is characterized by tunneling velocities smaller than v_0. In other words, the center of the tunneled wave packet falls behind the force-free one in this case, associated with a negative distance D in this regime.

The stationary-phase approximation allows in general for determination of the location x_p of a function $|\Psi(x)| \equiv |\int dk\, C(k) \exp[i\phi(k,x)]|$ at which it takes its maximum value. This peak value x_p is obtained from the condition $d\phi(k,x_p)/dk = 0$, where the derivative is evaluated where the (real) function $C(k)$ peaks, $k = k_p$. By Taylor expanding the phase ϕ as well as $C(k)$ around k_p one can see that a breakdown of this approximation is associated with nonzero third-order derivatives in $C(k)$ or ϕ. In the context of our situation, the function $C(k)$ corresponds to the product of the energy state amplitude and the absolute value of the transmission coefficient and $\phi(k,x)$, which is defined as $\alpha(k) + k(x - x_0) - E(k)T$. If we decrease the initial spatial width of the wave packet Δx, Δk increases and the function $C(k)$ becomes more asymmetric, and an increasing third-order derivative $d^3C(k)/dk^3$ will lead to a breakdown of the stationary-phase approximation. Equivalently, this breakdown can also be caused by an increase of the barrier width w, leading to an increase of the third-order derivative $d^3\phi(k)/dk^3$.

In order to demonstrate this breakdown of the stationary-phase approximation for larger barrier widths, we show in Fig. 2 similar graphs as in Fig. 1 but on a larger scale for the barrier width. We see that in the regime in which the barrier width w approaches the spatial width of the initial state Δx (which was chosen to be $\Delta x = 4$ a.u. in this simulation) the

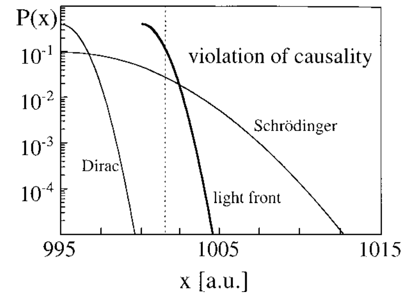

FIG. 3. The final spatial probability obtained from the solution of the Dirac and Schrödinger equations. The thick line is the light-cone probability as defined in the text. The parameters were $x_0 = -100$ a.u., $\Delta x = 1$ a.u., $v_0 = 136.411$ a.u., and $T = 8.027\,08$ a.u.

predictions of the analytical curves become less reliable. In fact, as we will demonstrate in Sec. II B, the definition of the spatial delay based on the peak value becomes meaningless.

Let us finish this section with a comment on the relation of superluminal speeds and the possible violation of Einstein's causality. We agree with the work of Chiao and coworkers, who point out that superluminal tunneling speeds are just a pulse-reshaping effect and therefore do not necessarily violate Einstein's causality. Other works [18] have argued that causality is not violated, because of the strong attenuation suffered by the transmitted signal. The special theory of relativity could be violated if the total spatial probability of the tunneled packet to find the particle to the right of position x, i.e., $\int_x^\infty dx |\Psi(x,T)|^2$, were larger than the corresponding probability for a fictitious wave packet that has moved with the speed of light c, i.e., $\int_x^\infty dx |\Psi(x - cT, T = 0)|^2$. The latter is defined by a wave packet that has been shifted from its initial position by the amount cT, where T is again the total time. Due to the relativistic suppression of spatial spreading first discussed in [19,20], the width of this ''light-cone'' packet is identical to its initial width Δx. A nonrelativistic theory, however, does not take this relativistic effect into account, and the wave front of a Schrödinger state with a relatively large initial speed close to c can actually exceed the integrated light-cone probability due to spreading, and therefore violate causality.

We demonstrate this violation of causality in Fig. 3 where we have evolved the same initial state with $v_0 = 136.411$ a.u. and $\Delta x = 1$ for $T = 8.027\,08$ a.u. using the Dirac and the Schrödinger theories. The thick line shows the light-cone probability. The sufficient condition for a violation of causality, $\int_x^\infty dx |\Psi(x,T)|^2 > \int_x^\infty dx |\Psi(x - cT, T = 0)|^2$, leads to $x > 1001.5$ a.u. for the (nonrelativistic) Schrödinger wave packet $\Psi(x,T)$. Clearly, causality is violated in the region $x > 1001.5$ a.u. for the nonrelativistic wave packet. On the other hand, the corresponding time-evolved wave function obtained from the Dirac equation is located entirely to the left of the light front and we have $\int_x^\infty dx |\Psi(x,T)|^2 < \int_x^\infty dx |\Psi(x - cT, T = 0)|^2$ for the entire spatial domain. The latter result can even be shown analytically [14]; the integral kernel associated with the free time Dirac evolution operator vanishes outside the light cone, therefore preventing any acausal behavior. In other words, if a spinor has a compact support in a finite domain of radius x,

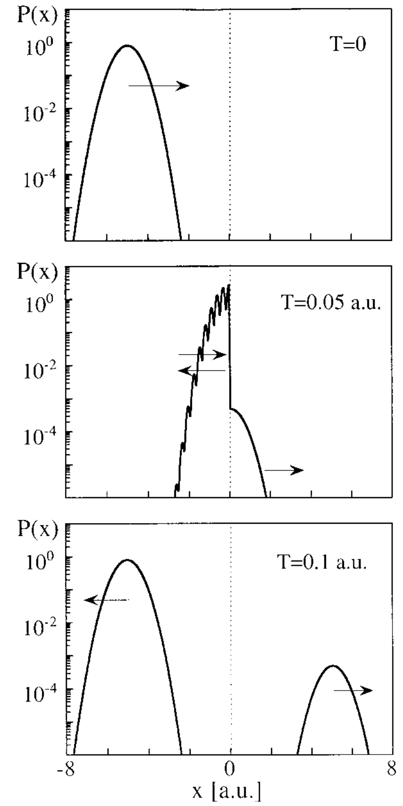

FIG. 4. The spatial probability density $P(x)$ before, during, and after scattering off a square potential barrier at times $T=0$, 0.05, and 0.1 a.u. The vertical dashed line indicates the location of the potential at $x=0$. The parameters were $x_0=-5$ a.u., $\Delta x=0.5$ a.u., $v_0=100$ a.u., $w=0.05$ a.u., and $W_0=1.5E_0$.

then at time T the state vanishes outside a domain of radius $x+cT$, which, of course, is not true for the Schrödinger equation.

To summarize, if tunneling is treated within the framework of the Dirac theory, causality cannot be violated in principle. This agrees with the conclusion [18,21] that the peak amplitude of the pulse emerging from the barrier is always lower than the amplitude that the pulse would have at the same instant of time if it were just propagating at c without attenuation.

B. Spatially narrow wave packets: $\Delta x<w$

As we have demonstrated in Fig. 2, if the spatial width Δx is of the same order as the width of the potential barrier w, the stationary-phase approximation becomes unreliable and one does not have the additional benefit of analytical approximations. In this regime the momentum scale on which the complex phase of the transmission amplitude varies, $\alpha/(d\alpha/dk)$, is larger than the momentum width of the wave packet. As a result, each momentum amplitude has a quite different complex phase and the superposition of the momentum states does not lead to a simple Gaussian-shaped spatial probability distribution as in the initial state. In fact, the spatial density of the transmitted pulse can be multipeaked with peak sizes varying as a function of time. In a space-time picture this could be interpreted as a kind of tunneling resonance. In fact, even the reflected density need not be describable by a simple spatial Gaussian. After the wave packet has tunneled through the barrier, its time evolution is described by that of a free particle whose center increases linearly in time independent of the spatial and temporal interference oscillations.

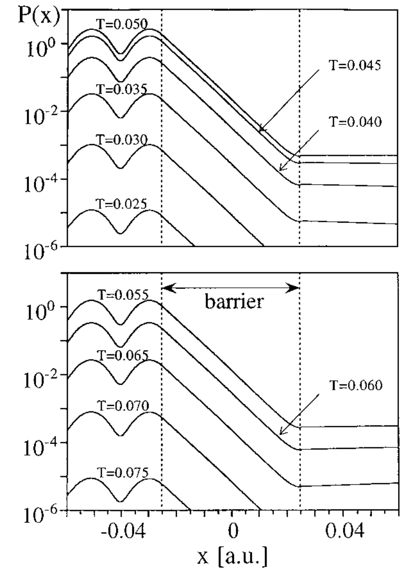

FIG. 5. The spatial probability density displayed in the spatial region near and inside the barrier at various times T in a.u. Same parameters as in Fig. 4.

III. TIME-RESOLVED TUNNELING UNDER THE POTENTIAL BARRIER

In this section we will analyze the tunneling process from a microscopic point of view. In Figure 4 we present snapshots of the spatial probability of the electron at initial, intermediate, and late times. As the initial wave packet was prepared to the left of the barrier, the probability density in the region $-w/2<x<w/2$ vanishes until the front edge of the incoming wave packet enters the barrier. Then the density grows and after the tunneling process it reduces back to zero. Clearly, at each time the density inside the barrier decreases monotonically as a function of x, as shown in Fig. 5. This stresses the point we made earlier that it is not trivial to trace directly the peak motion under the barrier. The almost parallel lines in the logarithmic plot for the region under the barrier indicate the exponential spatial decay. If these lines were actually precisely parallel, then the tunneling process could take place instantaneously in principle. The details of the incoming wave packet at $x=-w/2$ could then be instantaneously transmitted and copied over to the transmitted portion at $x=w/2$. On the other hand, we have shown in the previous section that the tunneling process does not happen instantaneously and requires a finite time associated with effective sub- or superluminal speeds.

As a side remark we should mention that, in contrast to the stationary solutions of the Schrödinger equation whose derivatives at $x=\pm w/2$ are continuous, the Dirac equation in principle permits its stationary solution to have a discontinuous derivative at the interfaces. Our time-dependent calculations, however, suggest that the wave-packet solution is actually smooth at these boundaries.

To investigate the mechanism of the tunneling in more detail, we have defined a quantity that will provide us with additional insight. For a given location x, we have computed numerically from our time-dependent wave function solution that specific time (which we denote by T_p) at which the spatial probability density $P(x,T)$ takes its maximum value:

$$\max \sum_{i=1}^{4} |\Psi_i(x,T)|^2 = \sum_{i=1}^{4} |\Psi_i(x,T_p)|^2. \tag{3.1}$$

Inside the barrier the wave function is certainly not spatially localized, as it always takes its spatial maximum at the left edge $x=w/2$, but it is *temporally localized* such that the peak time $T_p(x)$ can be unambiguously defined and calculated under the barrier as well. Before the wave packet arrives at the boundary, $T \ll (-x_0 - w/2)/v_0$, the function $T_p(x)$ is given by the linear dependence $T_p(x)=(x-x_0)/v_0$ for $x \ll -w/2$, if the wave-packet spreading is not significant [19,20]. Here the inverse value of the slope is the incoming velocity v_0.

In Fig. 6 we display the location x as a function of this temporal peak time (3.1) around and inside the barrier. For comparison we have indicated by the straight line the result obtained from a wave packet without any tunneling barrier, $x^{(0)}(T)=v_0 T + x_0$. There are two striking observations.

First, due to the details of the scattering process at the left edge of the barrier and the resulting interference of the incoming and reflected wave packets, the peak time for the tunneling case is actually different from that of the corresponding force-free wave packet at $x=-w/2$. For our chosen parameters, it turns out that this arrival time is actually *larger* than that associated with the free electron.

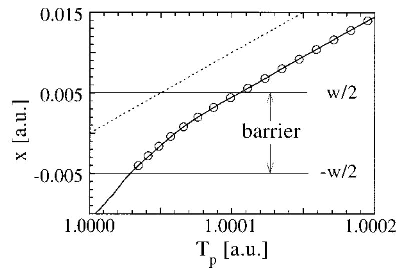

FIG. 6. The location x as a function of the temporal-peak time. The dashed line corresponds to the graph associated with a free wave packet in the absence of any scattering potential. The open circles denote the prediction according to the analytical formula based on the stationary-phase approximation [Eq. (3.4)]. The parameters were $x_0=-100$ a.u., $\Delta x=20$ a.u., $v_0=100$ a.u., $w=0.01$, and $W_0=1.5E_0$.

A second observation is about the region inside the barrier. We can define an *instantaneous* tunneling speed v_T as

$$v_T = \frac{1}{dT_p(x)/dx}, \tag{3.2}$$

which is a continuous function of the location x and whose value can be read off the graph.

For the special case of the square-well potential, the analytical form of the stationary states inside the potential is known and it is possible within the framework of the stationary-phase approximation to derive analytical formulas for this instantaneous tunneling velocity as a function of the distance:

$$\begin{aligned} 1/v_T &= dT_p(x)/dx \\ &= \frac{\kappa W_0 \Gamma B_1 \,\mathrm{sech}^2[\kappa(x-w/2)]\{1-\Gamma^2 \tanh^2[\kappa(x-w/2)]\}}{2\{1+\Gamma^2\tanh^2[\kappa(x-w/2)]\}^2} \\ &\quad + \frac{\Gamma B_2 \,\mathrm{sech}^2[\kappa(x-w/2)]\{1+\Gamma^2\tanh^2[\kappa(x-w/2)]-2\kappa(1+\Gamma^2)(x-w/2)\tanh[\kappa(x-w/2)]\}}{\kappa\{1+\Gamma^2\tanh^2[\kappa(x-w/2)]\}^2}, \end{aligned} \tag{3.3}$$

where

$$B_1 = \left[\frac{1}{E(W_0-E)} + \frac{1}{(E-W_0+2c^2)(E+2c^2)}\right]$$

and

$$B_2 = \left[-1 + \frac{(W_0-E)}{c^2}\right],$$

and where T_p is given by

$$T_p=\frac{\sqrt{1+k^2/c^2}}{k}\left(\frac{w}{2}-x_0\right)-\frac{w}{k}\left(1+\frac{E}{c^2}\right)+\frac{W_0(\Gamma^{-1}+\Gamma)B_1\tanh(\kappa w)+2w(\Gamma^{-1}-\Gamma)B_2\,\mathrm{sech}^2(\kappa w)}{4\{1+[(1-\Gamma^2)^2/4\Gamma^2]\tanh^2(\kappa w)\}}$$

$$+\frac{W_0\Gamma\kappa B_1\tanh[\kappa(x-w/2)]+2\Gamma B_2(x-w/2)\mathrm{sech}^2[\kappa(x-w/2)]}{2\kappa\{1+\Gamma^2\tanh^2[\kappa(x-w/2)]\}}. \quad (3.4)$$

To test the validity of the analytical formula (3.4), we have superimposed on the curve in Fig. 6 the predictions according to this formula (circles) for the Schrödinger theory, and the agreement is astonishing.

We should note that all analytical formulas derived in this section are based only on the first spinor component of the wave function. In the previous sections we have shown that this approximation works quite well for predicting the wave function outside the barrier region. However, inside the barrier the other spinor components are more important and the agreement between the exact peak time computed from all spinor components of the Dirac solution and its analytical approximation [Eq. (3.4)] is only qualitative and not as good as in the nonrelativistic case. We observed that, if the peak time was computed only from the first spinor component of the exact Dirac state, the analytical estimate of Eq. (3.4) (based on the first spinor) produces a relative error of less than $10^{-3}\%$.

Let us finish with a quick comparison of the effective tunneling speed v_e based on the spatial delay after the tunneling event with the instantaneous speed v_T introduced in Eq. (3.2). As an example, for the parameters discussed in the previous section ($x_0=-100$ a.u., $v_0=100$ a.u.) we found that the spatial delay was $D=-5.5\times10^{-3}$ a.u. for a wave packet that was associated with a temporal delay $\Delta T=-5.5\times10^{-5}$ a.u. Using Eq. (2.7) we associated this delay with an effective average tunneling speed of $v_e=64.5$ a.u. For these parameters, the graph in Fig. 6 shows that the center of the wave packet formed from the incoming and reflected waves reaches the left edge at the time $T_L=1.000\,030\,5$ a.u., which due to the interference is already delayed compared to the arrival time of a force-free wave packet ($T_L^{(0)}=0.999\,950\,0$ a.u.). Figure 6 also shows that the tunneled portion reaches the right edge $x=w/2$ at a time $T_R=1.000\,106\,8$ a.u. As a result, the time the electron has spent under the barrier is only $T_R-T_L=0.000\,076\,3$ a.u., which is shorter than the corresponding time $T_R^{(0)}-T_L^{(0)}=w/v_0=0.0001$ a.u. of the force-free electron. This time would amount to an average tunneling speed of $\overline{v_T}=w/(T_R-T_L)=131$ a.u. This average velocity $\overline{v_T}$ is much larger than the effective tunneling speed v_e calculated above in Sec. II. This huge difference (between 64.5 and 131 a.u.) is due to the delay of the wave function already present on the left edge of the barrier before the electron enters the potential. The speeding up of the particle under the barrier (associated with $\overline{v_T}=131$ a.u.) is compensated by the slowing down before entering the barrier, so that the effective speed that takes both mechanisms into account amounts to a net value of 64.5 a.u. We will present a more detailed discussion of the general properties of v_T elsewhere.

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