Relativistic analysis of a wave packet interacting with a quantum-mechanical barrier

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The dynamics of a wave packet incoming on a quantum-mechanical barrier is analyzed in the framework of a fully relativistic model, with particular emphasis on the case of a large spectrum. Some of the characteristic times of tunneling are calculated and compared; they are all of the same order of magnitude and all indicate an apparent superluminal motion, even if causality is maintained. A time-asymptotic expression for the transmitted wave function is derived and its strong validity is shown.

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I. INTRODUCTION

The problem of wave tunneling through a quantum-mechanical barrier has recently been reopened by the results of several experimental studies, which show a possible superluminal behavior of the wave packet [1–6]. The theoretical analysis of this phenomenon involves such general problems as the conservation of the concept of causality during the motion of the wave packet, but also more peculiar questions such as the definition and evaluation of the time spent by the packet inside the barrier. The features of wave tunneling were studied first by Wigner [7] and Hartman [8]. This latter author proposed an expression for the traversal time through the barrier which is valid for thin spectra. This time is usually called the phase time, and presents a saturation value for increasing barrier widths. The corresponding velocity should increase with this parameter and exceed the speed of light in vacuum. His original work, however, as well as most of the subsequent analyses [9–11], was based on the Schrödinger equation, which is not relativistic, and should, therefore, be inappropriate to describe the dynamics of a wave packet propagating at luminal or superluminal velocity. In this sense, there remain reasonable doubts that the superluminal behavior presented by the wave packet might be an artifact due to the inadequacies of the nonrelativistic model, rather than a real effect.

A few authors [12–14] have extended the analysis of the wave tunneling to a completely relativistic case, using the Dirac equation, which should be the natural tool to investigate the propagation of wave packets at large velocity. In some of this work [12,13], the authors describe the temporal evolution of a wave packet in the tunneling situation and demonstrate that it still presents superluminal behavior, even if the causality is fully restored.

In the present paper, we want to give a contribution in this direction. In Sec. II, we recall briefly the problem of propagation through a quantum-mechanical barrier by integration of the Dirac equation, analyzing in particular the regime of large-spectrum wave packets, which was studied by Krekora *et al.* but in less detail than the opposite regime. In Sec. III, we compute the time spent inside the barrier, making a comparison between the most common definitions of this quantity, namely, the Hartman phase time, the traversal time, and the dwell time [15,16]. In Sec. IV, we derive an original analytical estimate of the transmitted wave function and discuss the validity of this formula. Conclusions and comments are given in Sec. V.

II. PROPAGATION OF THE WAVE PACKET THROUGH THE BARRIER

The one-dimensional Dirac equation is commonly written as

$$i\frac{\partial\psi}{\partial t}=-ic\alpha_x\frac{\partial\psi}{\partial x}+c^2\beta\psi+V(x)\psi, \tag{1}$$

where α_x and β are the Pauli matrices, ψ is the two-component Dirac spinor, $V(x)$ is the potential, and atomic units ($e=\hbar=m_0=1$, $c=137$) are used. If the potential is a square barrier of height V_0 and width a, using a standard technique we obtain the stationary solutions of the equation. For instance, if a wave packet approaches the barrier from the left, in the region at the right of the barrier the stationary solution can be written as

$$u(x)=\mathrm{F}e^{ipx},$$

where $cp=(E^2-c^4)^{1/2}$, E being the total energy and F the two-component spinor

$$\frac{F}{A}=\begin{pmatrix}1\\ \sqrt{\dfrac{E-c^2}{E+c^2}}\end{pmatrix}\frac{4\gamma pp'e^{-ipa}}{(p+\gamma p')^2e^{-ip'a}-(p-\gamma p')^2e^{ip'a}}, \tag{2}$$

where $\gamma=(E-c^2)/(E-c^2-V_0)$, $cp'=[(V_0-E)^2-c^4]^{1/2}$ is the momentum of the particles inside the barrier, and $A(p)$ is the initial spectrum of the wave packet.

By analysis of the quantity p', we recall briefly that propagation through the barrier occurs when $E>V_0+c^2$ or when $c^2<E<V_0-c^2$. This last region of propagation (where the phenomenon called Klein tunneling takes place [17]) exists only if $V_0>2c^2$. In the intermediate region, namely, for $V_0-c^2<E<V_0+c^2$ ($c^2<E<V_0+c^2$, if V_0

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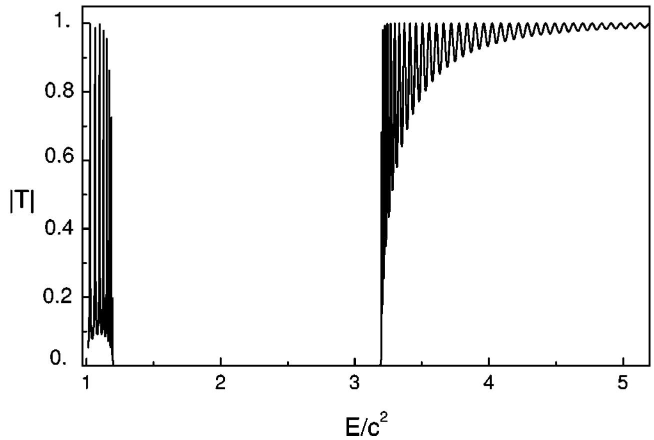

FIG. 1. Modulus of the complex coefficient of transmission $|T|$ versus energy E/m_0c^2, for $a=0.3$ and $V_0/m_0c^2=2.2$.

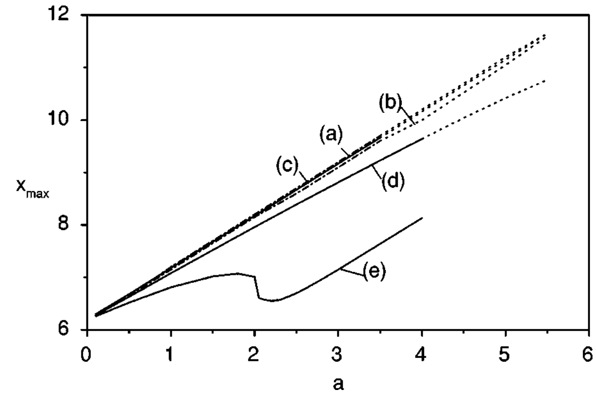

FIG. 2. Position of the peak of the wave function x_{max} versus the barrier width a at $t=0.1$ for $p_0=146$, $V_0/m_0c^2=1.5$, and $\Delta p_0=$(a)0.5, (b) 2.0 (dashed lines), and $V_0/m_0c^2=2.2$ with $\Delta p_0=$(c)0.5, (d) 2, and (e) 3.5 (solid lines). The dotted parts of the lines correspond to situations where the average values are superluminal.

$<2c^2$) the wave inside the barrier is evanescent and the phenomenon of tunneling takes place. This is shown, for a potential $V_0/c^2=2.2$, in Fig. 1, where the transmission coefficient $|T|=|F/A|$ is presented as a function of E/c^2 for a barrier width $a=0.3$. The presence of geometrical resonances produces oscillations of $|T|$ in both regions of transmission. If the potential V_0 is greater than $2c^2$, the analysis of the step of the potential yields a paradoxical value of the reflection coefficient greater than 1, or, provided p is negative, to a nonvanishing value of the transmission coefficient when V_0 tends to infinity. This is the so-called Klein paradox [17], reconsidered by Telegdi [18] and resolved by Hansen and Ravndal [19] by admitting that the potential step emits electron-positron pairs. The analysis of the potential barrier made by Calogeracos and Dombey [20] shows that the emission of particles from the barrier is a transient phenomenon, occurring during the growth phase of the potential. In the following, when cases with $V_0>2c^2$ are concerned, we consider a scenario where the potential is adiabatically switched on from zero, and the wave packet is injected onto the barrier only when the particle emission occurring in this first phase is completely concluded.

The temporal evolution of the wave packet can be obtained by reconstructing the wave function in its integral form:

$$\psi=\int dE\, F(E)e^{i\sqrt{E^2-c^4}x/c-iEt}. \tag{3}$$

In the tunneling situation, superluminal behavior can be found. In fact, temporal analysis of the wave-packet dynamics shows that the transmitted wave packet, at least in some situations, emerges from the barrier before the corresponding wave packet that travels freely in vacuum, accumulating therefore a space advance. The space advance depends on the width of the barrier a as shown in Fig. 2, where the position of the peak of the wave packet x_{max} is shown versus a for a fixed time and for a Gaussian spectrum centered at $p_0=146$, with various values of the spread in momentum Δp_0 and for two different values of the potential V_0, the first one $V_0/c^2=1.6$ [curves (a) and (b)] and the second one $V_0/c^2=2.2$. The advance can increase regularly, as for instance in curves (a) ($\Delta p_0=0.5, V_0/c^2=1.6$), (b) ($\Delta p_0=5.0, V_0/c^2=1.6$), (c) ($\Delta p_0=0.5, V_0/c^2=2.2$), and (d) ($\Delta p_0=2.0, V_0/c^2=2.2$). It can sometimes be so large that the apparent velocity of translation of the wave packet is found larger than c. Although the theory used is fully causal, the average values sometimes show superluminal behavior. This situation is usually referred to as a behavior of weak causality [21,22].

In Fig. 2, the analysis has been carried out at a time $t=0.1$, which is sufficiently short to permit of obtaining mean velocities (calculated over the whole spatial interval traveled by the wave packet, which is considerably wider than the barrier width) larger than c. The range of the parameters where this situation occurs is evidenced in the figure by dotted curves. For instance, we have that a wave packet starting at $t=0$ at $x_0=-3.8$, traveling with a velocity $v=c=137$, will be at $t=0.1$ in the position $x=9.9$. All the situations where the packet is, at this same time, beyond this position, are characterized by a mean velocity, averaged over the whole temporal period considered, larger than c. In this analysis, we compare the position of the peak of the wave packet at $t=0.1$ with its position at $t=0$, and we evaluate the mean velocity in this interval. Since the wave packet presents interference fringes in the neighborhood of the barrier, this comparison can be used to evaluate a mean velocity only if at the initial and at the final instants considered the wave packet is sufficiently far from the barrier, in such a way that the interference process is not yet begun or is completely ended.

As can be seen from Fig. 2, the spatial advance increases regularly for $V_0/c^2=1.5$ for all values considered of Δp_0; in the case $V_0/c^2=2.2$ this monotonic increase takes place only for thin spectra. In this range of potential, for a wave packet with a large spectrum, a region of less pronounced advance with respect to the free propagation takes place when $\Delta x \approx a$ [see curve (e), in which $\Delta p_0=3.5$]. This is due to the fact that, when the spectrum is broad, the tail of the momentum distribution invades the Klein transmission region at low values of energy ($E<V_0-c^2$), and these slower components

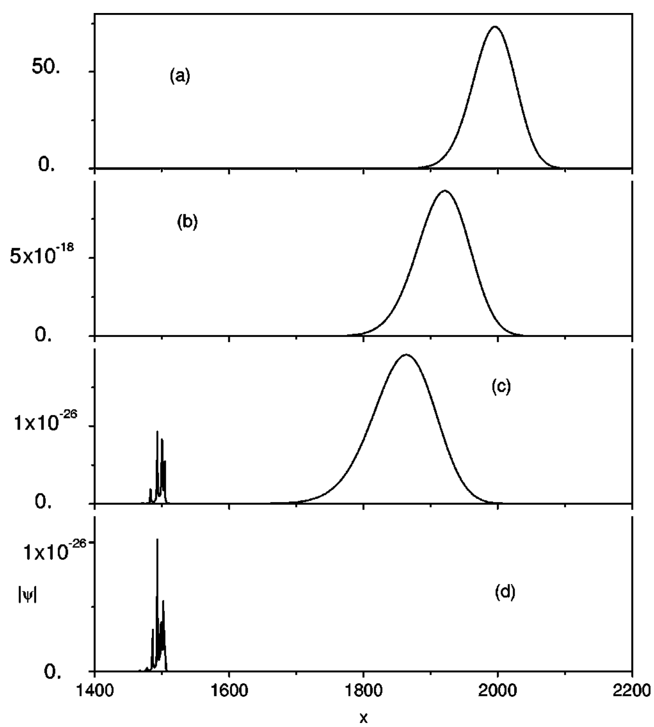

FIG. 3. Modulus of the wave function $|\Psi|$ (in arbitrary units) versus x at $t=20$ for $p_0=146$ $V_0/m_0c^2=2.2$, $\Delta p_0=5$ and $a=$(a)0.01, (b) 0.5, (c) 0.75, and (d) 1.

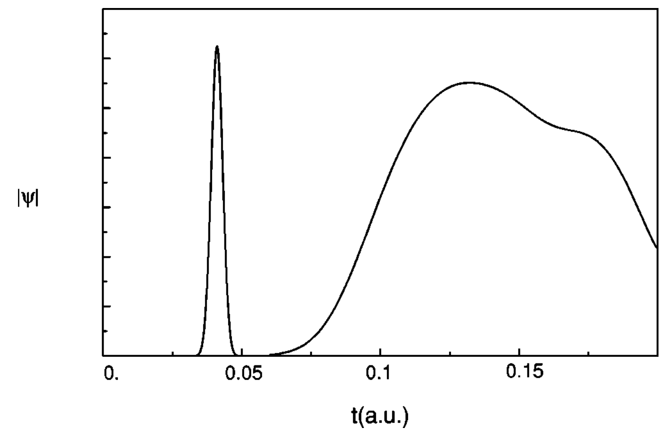

FIG. 4. Modulus of the wave function $|\Psi|$ (in arbitrary units) versus t at $x=a$, for $a=0.78$, $p_0=146$, $V_0/m_0c^2=2.2$, $\Delta p_0=5$.

compete with the faster ones, becoming progressively dominant as the barrier width increases. For thin spectra, instead, the transmitted wave packet maintains the Gaussian shape without distortions and the peak value decreases strongly with increasing barrier width. In all cases where $V_0/c^2>2$, the incidence of the wave packet onto the barrier must occur after a time interval $t=(a/c)[V_0/(2c^2)-1]^{-1/2}$ with respect to the switch-on of the barrier itself [20], in order to permit the conclusion of the particle emission process. In Fig. 3, the dynamics of the transmitted wave packet is shown in the case of a large spectrum and high potential, with $\Delta p_0=5$, and for various increasing values of the width of the barrier a. The analysis is made at a time sufficiently large ($t=20$) to permit clear separation between the slow and the fast components. For a very thin barrier [curve (a), $a=0.01$], the wave packet is strongly superluminal in the region of the barrier and the peak is therefore advanced with respect to the free propagation of a quantity $\delta x=0.66$. For more opaque barriers the superluminality cannot be revealed from this snapshot and the peak at this time shows a delay [curve (b), $a=0.5$]. The formation of two distinct wave packets is shown in curve (c) ($a=0.75$). The leading part, which is more advanced, derives from the tunneling, maintains the Gaussian shape, and decreases strongly with increasing a. The trailing part derives from the low-momentum transmission and its shape is determined by the presence of geometrical resonances. The curve (d) ($a=1.0$) shows the case where the tunneled part is considerably smaller than the transmitted one and the leading tail of the transmitted part masks the tunneling completely. This fact is apparent also in the temporal analysis. In Fig. 4 $|\psi|$ is presented for $x=a$ versus time and for $\Delta p_0=5$, $a=0.78$. The peak of the wave packet arrives at $x=0$ at $t\approx 0.038$. The sequence of two temporal maxima, the first one superluminal, the second one retarded, is clearly shown. The conclusions that can be drawn from comparison of the data of Figs. 3 [curve (c)] and 4 (which are made with only slightly different data) are not contradictory. The superluminality of the first peak of Fig. 4 at $t=0.041$ (evaluated as $v\approx a/[t(x=a)-t(x=0)]\approx 1.8c$) is reabsorbed at subsequent times just because the components of the spectrum with low momentum slow down the whole wave packet. The presence and the effects of the tail on the momentum distribution could be avoided by cutting off the spectrum or by choosing the initial parameters of the wave packet in a suitable way, for instance, by eliminating the Klein transmission range with a potential value $V_0<2c^2$.

III. TUNNELING TIMES

The characteristic time in which the phenomenon of tunneling through a barrier takes place can be evaluated with the Hartman phase time calculated, for the Dirac equation, by Krekora *et al.* [12,13]. The limiting value of t_H for $a\gg 1$ is given by $t_H=(2E-V_0)/(c^2pp')$. The Schrödinger equation gives, instead, for this same limit, the value $t_H=V_0/c^2pp'$, where $p=\sqrt{2E}$ and $p'=\sqrt{2(V_0-E)}$. If we compare a relativistic and a nonrelativistic packet with the same kinetic energy, the delay time for the relativistic wave packet is shorter than the classical one for lower energies, while for higher energies the classical packet transits in a shorter time, according to the results of Ref. [13]. In any case the differences are always very small and the order of magnitude of these two times always remains the same, as reported in Fig. 5, where the relativistic limit [curve (a)] and the classic one [curve (b)] are presented as functions of E/m_0c^2. Another characteristic time is commonly constructed by recording the instants τ_{in} and τ_{fin} of the passage of the wave-packet maximum through the initial and final points of the barrier, and calculating the difference $\tau_{\text{tr}}=\tau_{\text{fin}}-\tau_{\text{in}}$. It is important to note that, even if the interference between the transmitted and the reflected packets does not

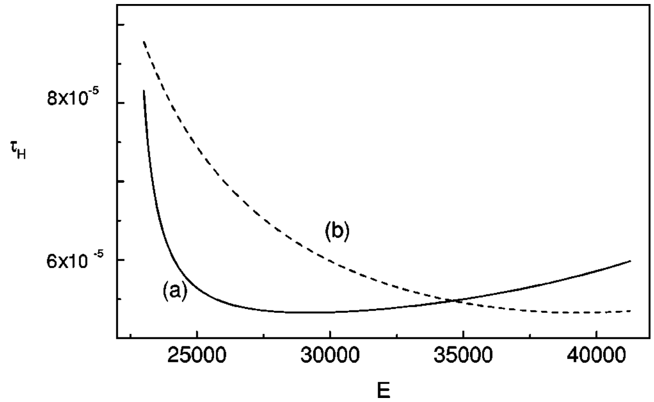

FIG. 5. Limit for $a \gg 1$ of the Hartman phase time in the nonrelativistic (dotted line) and relativistic (solid line) model for $V_0/m_0c^2 = 2.2$

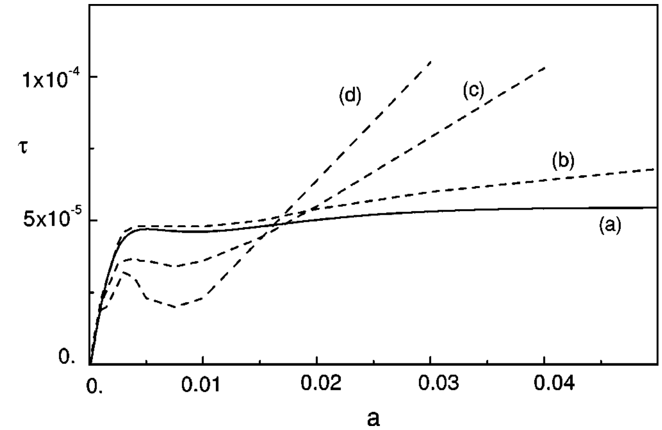

FIG. 7. Curve (a): Hartman phase time τ_H versus a for $E/m_0c^2 = 1.46$ and $V_0/m_0c^2 = 2.2$. Traversal time $\tau_{\rm tr}$ versus a for $\Delta p_0 = 2$ [curve (b)], 5 [curve (c)], and 8 [curve (d)].

permit one to record a spatial maximum of the wave packet due to the presence of the fringes, the variation in time of the distribution of probability at a fixed position is bell shaped, always without fringes, and this behavior permits one to determine precisely the transit time of the wave-packet maximum. In Fig. 6 the traversal time $t_{\rm tr}$ is reported as a function of a for various values of Δp_0, and compared with the phase time [curve (a)] for $p_0 = 146$ and $V_0/c^2 = 1.5$. Even for relatively thin spectra [curve (b), with $\Delta p_0 = 2.0$], the traversal time does not agree with the delay time, being always considerably shorter, and this disagreement increases for thicker barriers. For large spectra [curve (c) with $\Delta p_0 = 8.0$ and curve (d) with $\Delta p_0 = 15$], the monochromatic analysis given by Hartman is no longer valid, and the deviations of the traversal time with respect to the phase time are strong. In Fig. 7 the phase [curve (a)] and the traversal times are presented again for another set of parameters: $V_0/c^2 = 2.2$ and $\Delta p_0 = 2.0$ [curve (b)], 5.0 [curve (c)], and 8.0 [curve (d)]. In this case, the deviations of the traversal time with respect to the phase time are in two directions. For large barriers, the slow components prevail, and the signal appears retarded, as already shown in the previous section. For thin barriers, instead, the signal is strongly accelerated; it can even occur that the outgoing peak appears before the incoming peak enters. Situations of this kind, which are usually ascribed to the reshaping of the wave packet in traveling through the barrier, are shown in Fig. 8 where $\tau_{\rm tr}$ is plotted vs Δp_0 for $a = 0.0075$ and $V_0/c^2 = 2.2$ [curve (a)], for $a = 0.03$ and $V_0/c^2 = 2.2$ [curve (b)], and for $a = 0.015$ and $V_0/c^2 = 1.5$ [curve (c)]. The quantity $\tau_{\rm tr}$, for the case of the narrower barriers, becomes negative for increasing Δp_0 for both the potentials considered. This regime is, however, limited to a very small region in the parameter space. In fact, in the case $V_0/c^2 = 2.2$ and for barriers a little thicker [curve (b) with $a = 0.03$] the situation is already different, and the traversal time is positive and larger than the phase time, indicating the prevalence of the slow component.

One of the characteristic times of the interaction between the wave packet and the barrier is the dwell time [23], defined in its simplest form as

$$\tau_D = \int dt \int_0^a dx |\psi|^2. \tag{4}$$

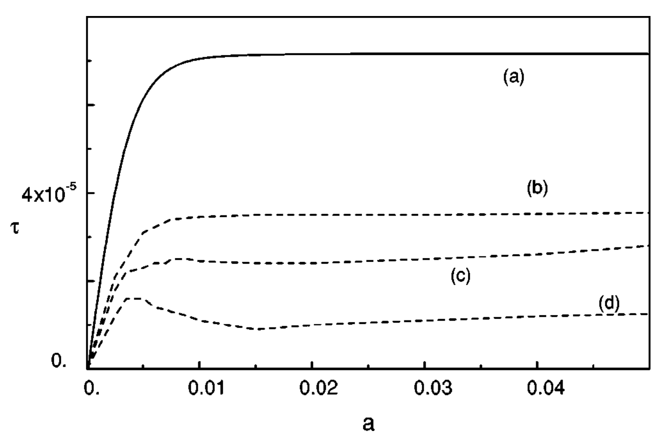

FIG. 6. Curve (a): Hartman phase time τ_H versus a for $E/m_0c^2 = 1.46$ and $V_0/m_0c^2 = 1.5$. Traversal time $\tau_{\rm tr}$ versus a for $\Delta p_0 = 2$ [curve (b)], 8 [curve (c)], and 15 [curve (d)].

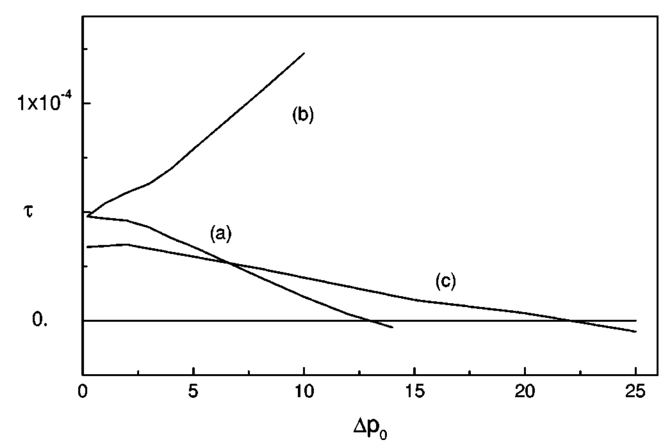

FIG. 8. Traversal time $\tau_{\rm tr}$ versus Δp_0 for (a) $V_0/m_0c^2 = 2.2$, $a = 0.0075$; (b) $V_0/m_0c^2 = 2.2$, $a = 0.03$; and (c) $V_0/m_0c^2 = 1.5$ and $a = 0.015$.

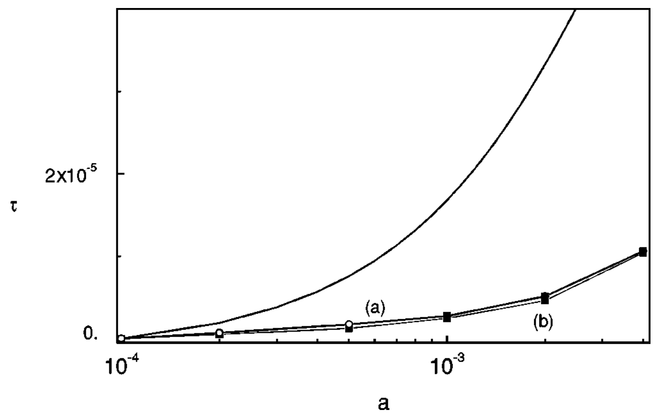

FIG. 9. Dwell time τ_D for $\Delta p_0=5.0$ (open circles) and 0.5 (solid squares) and for $E/m_0c^2=1.46$ and $V_0/m_0c^2=1.5$. Phase time for the same values of potential and energy.

It represents the time of permanence of the wave packet inside the barrier. We should note, however, that the use of expression (4) to give an estimate of the tunneling time must be limited to those cases where the reflection is actually negligible. In Fig. 9 the dwell time is represented, for the relativistic model, as a function of a, for $V_0/c^2=1.5$ and for $\Delta p_0=5$ [curve (a)] and 0.5 [curve (b)]. The phase time is also represented for comparison. For all cases shown, the transmission is larger than 97%, so that we can assume the full validity of the definition (4). The dwell time in all these cases turns out to be shorter than the phase times, and it is rather independent of the spread in momentum. This characteristic time also shows therefore a superluminal behavior.

IV. ANALYTICAL EXPRESSION OF THE WAVE FUNCTION

In the transmission region, the components of the wave function are represented by the integral (3), where F has been defined as expression (2) in Sec. II, and A, appearing in F, is the initial spectrum of the wave packet.

We consider, for the sake of simplicity, only the first component ψ_1 of the spinor and all the considerations that will be made must be repeated for the other component ψ_2.

The integral form (3) can be treated in the limit $t \gg E$ with the method of the stationary phase [24], because the phase $\phi=\sqrt{E^2-c^4}(x-a)/c-Et$ has a stationary point for the value $E=\tilde{E}=c^3t/\sqrt{c^2t^2-(x-a)^2}$.

Calling $\zeta=\sqrt{c^2t^2-(x-a)^2}$, a quantity connected with the distance between the position examined and the light front, the value of the stationary point can be written as $\tilde{E}=c^3t/\zeta$, and the corresponding value of the phase is $\phi(\tilde{E})=-c\zeta$.

The first component of the wave function can then be approximated by the expression

$$\psi_1=\sqrt{2\pi}\frac{xc^{3/2}}{\zeta^{3/2}}F\left(c^3\frac{t}{\zeta}\right)e^{-ic\zeta-i\pi/4}, \qquad (5)$$

where

$$F\left(\frac{c^3t}{\zeta}\right)=\frac{A(cx/\zeta)e^{-icxa/\zeta}}{\cos(p'a)-2i\Theta\sin(p'a)}E,$$

$$cp'=\sqrt{\left(V_0-\frac{c^3t}{\zeta}\right)^2-c^4},$$

and

$$\Theta=\frac{c^2x^2-V_0ct\zeta}{2x\sqrt{(\zeta W_0-c^3t)^2-c^4\zeta^2}}.$$

The quantity $A(cx/\zeta)$ is the initial spectrum of the wave packet, calculated at the value $p=cx/\zeta$. If the wave spectrum is Maxwellian, it is written as

$$A(cx/\zeta)\approx e^{-(cx/\zeta-p_0)^2+icxx_0/\zeta}.$$

Furthermore, if most of the spectrum falls in the tunneling range and if $|p'a|\gg 1$ we can simplify the factor $F(\tilde{E})$ in the form $F(\tilde{E})=[4A(\tilde{E})\gamma pp'/(p+i\gamma|p'|)^2]e^{ipa-|p'|a}$ and finally get

$$|\psi_1|=\sqrt{\frac{\pi c}{2}}\frac{cx^2-V_0t\zeta}{\zeta^{3/2}\sqrt{(\zeta V_0/c^2-ct)^2-\zeta^2}}\times e^{-(cx/\zeta-p_0)^2/(2\sigma_p^2)-|p'|a}. \qquad (6)$$

A numerical comparison between the complete (3) and the approximate expression (6) performed for the modulus of the wave function $|\psi|=\sqrt{|\psi_1|^2+|\psi_2|^2}$ shows the strong validity of the analytical expression. In fact, in the tunneling condition, the two forms essentially coincide even at very short times ($t=0.5$) as shown in Fig. 10, where $|\psi|$ is shown versus x for $a=0.1$, $\Delta p_0=5$ (complete form, dashed line, and asymptotic form, solid line) at $t=$(a) 0.1 and (b) 0.5. If the spectrum is centered in the Klein region, and there is therefore a strong contribution from the transmission regions, the asymptotic form is always valid, but after a longer time. This situation, which we present for its mathematical interest as a test for the validity of the asymptotic expansion, is reported in Fig. 11 ($a=5$, $\Delta p_0=1$, $V_0/m_0c^2=5$, and $p_0=50$). Substantial coincidence between the complete and the asymptotic forms is reached at $t=500$ (b). This is due to the fact that, for the complete validity of the approximate expression, there must not be tails of the wave function inside the barrier. The geometrical resonances present in the transmission region cause a bounce motion of the wave packet inside the barrier, which enhances the permanence time of the particles.

V. CONCLUSIONS

The relativistic dynamics of a wave packet incoming on a quantum-mechanical barrier has been analyzed by means of the Dirac equation, which should be the most appropriate

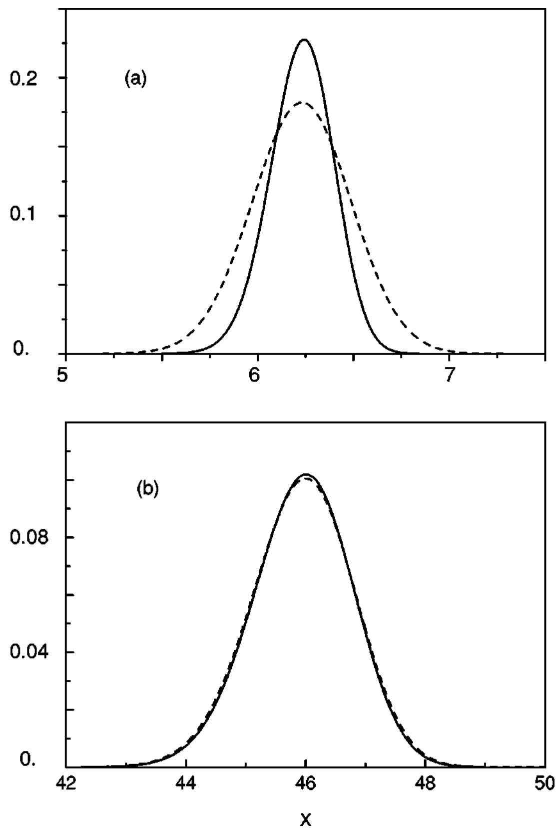

FIG. 10. Comparison between the complete integral form of the wave function (dotted line), and the asymptotic form (solid curve) in arbitrary units for $a=0.1$, $\Delta p_0=5.0$, $V_0/m_0c^2=2.2$, $p_0=146$, and $t=$(a)0.1 and (b) 0.5.

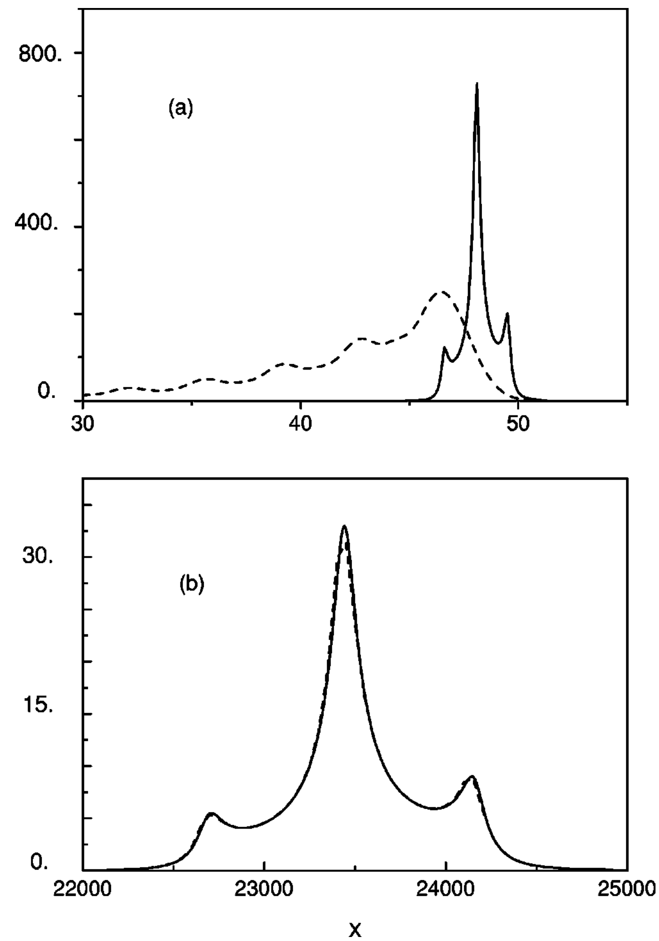

FIG. 11. Comparison between the complete integral form of the wave function (dotted line) and the asymptotic form (solid curve) in arbitrary units for $a=5$, $\Delta p_0=1.0$, $V_0/m_0c^2=5.0$, $p_0=50$, and $t=$(a)1 and (b) 500.

tool for the study of an energetic wave packet. The principal conclusions that we can draw are that the nonrelativistic analysis based on the Schrödinger equation gives results that, although coming from a theory that does not respect the causality, are qualitatively in substantial agreement with the relativistic ones. In particular, in the relativistic framework, we also recover the superluminal behavior of the wave packet, already found with the Schrödinger model. This behavior must be considered therefore not as an artifact connected to the use of an inadequate model, but as an effect compatible with the precepts of causality and of relativity. We agree with the conclusion of Ref. [12] also in finding that, in some conditions, the superluminal behavior predicted by the Dirac model is more accentuated than in the nonrelativistic one. We have extended the analysis to broad-spectrum wave packets. In this condition, there can be a contribution from the slow components of the spectrum, falling in the Klein transmission region, that alters the tunneling phenomenon. In general, the superluminality disappears in this condition, except in the case of a very thin barrier, where the appearance of the tunneled peak beyond the barrier can even anticipate the entrance of the incoming wave packet, leading to negative traversal times. The superluminality may depend on the shape of the potential, and in particular on the presence of a sharp discontinuity or on the value of the spatial gradient of the potential. This behavior could be analyzed using, for instance, the Woods-Saxon potential barrier which has been analytically solved [25]. Another characteristic time, namely, the dwell time, which is positive by definition, and which is connected to the permanence of the particles inside the barrier, gives for the tunneled packet traversal velocities larger than c. It turns out to be independent of the spread in momentum and to reach a saturation value for increasing barrier width, showing therefore a behavior similar to that of the Hartman phase time.

Finally, we derived an analytical expression for the wave function in the transmission region for very large times. A comparison between the approximate and complete forms shows the strong validity of the asymptotic expression in all the different regimes considered.

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