Early times in tunneling

Gastón García-Calderón

Instituto de Física, Universidad Nacional Autónoma de México
Apartado Postal 20-364, 01000 México, D.F., México

Jorge Villavicencio

Facultad de Ciencias, Universidad Autónoma de Baja California
Apartado Postal 1880, Ensenada, B.C., México

(20 June 2000)

Exact analytical solutions of the time-dependent Schrödinger equation with the initial condition of an incident cutoff wave are used to investigate the traversal time for tunneling. The probability density starts from a vanishing value along the tunneling and transmitted regions of the potential. At the barrier width it exhibits, at early times, a distribution of traversal times that typically has a peak $\tau_p$ and a width $\Delta \tau$. Numerical results for other tunneling times, as the phase-delay time, fall within $\Delta \tau$. The Büttiker traversal time is the closest to $\tau_p$. Our results resemble calculations based on Feynman paths if its noisy behaviour is ignored.

PACS numbers: 03.65.Bz, 03.65.Ca, 73.40.Gk

Quantum tunneling, that refers to the possibility that a particle traverses through a classically forbidden region, constitutes one of the paradigms of quantum mechanics. In the energy domain, where one solves the stationary Schrödinger equation at a fixed energy $E$, tunneling is well understood. In the time domain, however, there are aspects still open to investigation. Recent technological achievements as the possibility of constructing artificial quantum structures at nanometric scales [1] or the manipulation of individual atoms [2] have stimulated work on time-dependent tunneling both at applied and fundamental levels. A problem that has remained controversial and the subject of a great deal of attention over the years is the tunneling time problem [3], that can be stated as the question: How long it takes to a particle to traverse a classically forbidden region? In time-dependent tunneling, many works attempting to answer the above question consider the numerical analysis of the time-dependent Schrödinger equation with the initial condition of a Gaussian wave packet [4,9,10]. A common feature of the majority 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 and hence usually it is required a long time analysis of the solutions. The above situation may be circumvented by considering cutoff wave initial conditions [11,12,13,14,16].

In this work we consider a analytic time-dependent solutions to the Schrödinger equation with the initial condition at $\tau = 0$ of a incident cutoff wave, to investigate the traversal time for tunneling through a potential barrier. The problem may be visualized as a gedanken experiment consisting of a shutter, situated at $x = 0$, that separates a beam of particles from a potential barrier of height $V_0$ located in the region $0 \leq x \leq L$. At $\tau = 0$ the shutter is opened. The probability density rises initially from a vanishing value and evolves with time through $x > 0$. At the barrier edge $x = L$, the probability density at time $\tau$, yields the probability of finding the particle after a time $\tau$ has elapsed. Since initially there is no particle along the tunneling region, detecting the particle at the barrier edge at time $\tau$, provides a measure of its traversal time through the tunneling region.

The transient behavior of the time-dependent solution at early times and at distances close to the interaction region plays a significant role in our approach. Other formulations, based on the stationary solutions of the Schrödinger equation [11,12], refer to asymptotically long times at large distances and hence ignore transient effects. These approaches provide a single value for the traversal time. In contrast, our approach leads to a distribution of traversal times as in works based on the Feynman path integral method [11,12], though as indicated below both approaches differ in important aspects.

In a recent paper we have obtained the time-dependent solution to the Schrödinger equation for tunneling through an arbitrary potential of finite range with the initial condition of a cutoff plane wave of momentum $k$. The solution may be written as a term proportional to the free solution plus a contribution involving an infinite sum of resonance terms associated with the $S$–matrix poles of the potential [11]. Our approach is based on the Laplace transform technique and considers some analytical properties of the outgoing wave propagator. Some
decades ago Moshinsky considered the free case solution to the above problem \[11\]. Moshinsky showed that the probability density, for a fixed value of the distance \(x_0\) as a function of \(t\), exhibits a transient regime that he named diffraction in time. Recently, observations of that phenomenon have been reported \[7\]. For the sake of simplicity in our approach, as Moshinsky also did, 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 becomes more involved \[13\]. As shown below the terms depending on the \(S\)–matrix poles provide a novel transient behavior that may dominate the early times in the tunneling process.

The plane wave cutoff initial condition discussed in Refs. \[12,14\] 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,

\[
\psi_s(x, k, \tau = 0) = \begin{cases} 
  e^{ikx} - e^{-ikx}, & x < 0 \\
  0, & x > 0.
\end{cases}
\]  

(1)

One can then proceed along lines similar to those discussed in Ref. \[9\] to derive the time-dependent solution \(\psi_s(x, k, \tau)\) of the Schrödinger equation for a potential \(V(x)\) that vanishes outside the region \(0 \leq x \leq L\). The solution along the internal region reads,

\[
\psi_s(x, k, \tau) = \phi(x, k)M(0,0,k,\tau) - \phi(x,-k)M(0,-k,\tau)
- \sum_n \phi_n(x)M(0,k_n,\tau), \quad (0 \leq x \leq L)
\]

(2)

where \(\phi(x,k)\) refers to the stationary solution and \(\phi_n(x) = 2iku_n(0)u_n(x)/(k^2 - k_n^2)\) is given in terms of the resonant (Gamow) states \(\{u_n(x)\}\) and complex poles \(\{k_n\}\) of the problem \[10,14\]. Similarly the transmitted solution \[13\] becomes,

\[
\psi_s(x, k, \tau) = T(k)M(x, k, \tau) - T(-k)M(x, -k, \tau)
- \sum_n T_n M(x,k_n,\tau), \quad (x \geq L)
\]

(3)

where \(T(k)\) and \(T(-k)\) are transmission amplitudes, and \(T_n = 2iku_n(0)u_n(L)\exp(-ikL)/(k^2-k_n^2)\). In the above two equations the functions \(M(x, k, \tau)\) and \(M(x, k_n, \tau)\) are defined as,

\[
M(x, q, t) = \frac{1}{2}e^{i(mx^2/2\hbar\tau)}e^{iy^2/\hbar^2}erfc(y_q);
\]

(4)

where the argument \(y_q\) is given by

\[
y_q = e^{-in} \frac{m}{2\hbar^2} \left[ \frac{x - \bar{q}n}{m} \right].
\]

(5)

In Eqs. (3) and (4) \(q\) stands either for \(k\) or \(k_n\), the index \(n\) refers to a given complex pole. Poles are located on the third and fourth quadrants of the complex \(k\)-plane. The solution for the free case with the reflecting initial condition is, \(\psi_s^0(x, k, \tau) = M(x, k, \tau) - M(x, -k, \tau)\). From the analysis given in Ref. \[13\] one can see that the above exact solutions satisfy the corresponding initial conditions, i.e., they vanish exactly for \(x > 0\). At very long times it is also shown in Ref. \[13\] that the terms \(M(x, k_n, \tau)\) that appear in the above equations vanish. The same occurs for \(M(x, -k, \tau)\) while, as shown firstly in Ref. \[11\], \(M(x, \pm k, \tau)\) tends to the stationary solution. Hence, at long times, each of the above exact solutions go into the corresponding stationary solutions, namely, along the internal region as \(\psi(x, \tau) = \phi(x,k)\exp(-iE\tau/\hbar)\) and along the external region as \(\psi(x, \tau) = T(k)\exp(ikx)\exp(-iE\tau/\hbar)\). Note that at early times and short distances there is a competition between the contribution of the free-type terms (\(M\) functions depending on \(k\)) and the pole terms (\(M\) functions depending on either \(k_n\) or \(k_{-n}\)) in Eqs. (3) and (4). As exemplified below, depending on the potential parameters one may have the predominance of one or the other type of terms. Note also that the initial state is not strictly monochromatic (it extends from \(-\infty\) to \(0\)) and hence it has a distribution of components around \(k\) in momentum space. One could construct an initial cutoff wavepacket as a linear combination of cutoff waves. However, since we compare below with definitions of tunneling times involving plane waves, wavepackets will not be considered here. Besides, in general they involve no negligible momentum components above the barrier potential and hence obscure the dynamics of tunneling.

In order to apply the above ideas, we consider a model that has been used extensively for the tunneling time problem, namely, the rectangular barrier potential, characterized by a height \(V_0\) in the region \(0 \leq x \leq L\). The shutter is located at \(x = 0\). In order to calculate Eqs. (2) and (3) for the initial condition (1), in addition to the parameters \(V_0, L\), and that corresponding to the incident energy \(E = \hbar^2 k^2/2m\), we need to determine the complex poles \(\{k_n\}\) and resonant states \(\{u_n(x)\}\). It is well known that for a finite range potential there are an infinite number of poles. The \(S\)-matrix poles for the rectangular barrier potential may be obtained from the corresponding transmission amplitude \(T(k) = 4kq\exp(-ikL)/J(k)\), where \(q = [k^2-k_0^2]^{1/2}\) with \(k_0^2 = 2mV_0/\hbar^2\). They correspond to the zeros of \(J(k)\) in the \(k\)-plane, namely,

\[
J(k) = (q+k)^2\exp(-iqL) - (q-k)^2\exp(iqL) = 0.
\]

(6)

We follow a well established method to obtain the solutions to the above equation \[14,22\]. The resonant states of the problem satisfy the time-independent Schrödinger equation of the problem with outgoing boundary conditions \[16\]. They read,

\[
u_n(x) = C_n [a e^{iq_n x} + b_n e^{-iq_n x}], \quad (0 \leq x \leq L)
\]

(7)

where \(b_n = (q_n + k_n)/(q_n - k_n)\) and \(C_n\) may be obtained from the normalization condition \[13\].
\[
\int_0^L u_n^2(x)dx + i \frac{u_n^2(0) + u_n^2(L)}{2k_n} = 1.
\] (8)

Note that both the complex poles and the resonant states are a function of \(V_0\) and \(L\) and hence are a property of the system.

To exemplify the time evolution of the probability density we consider the set of parameters: \(V_0 = 0.711\ eV, L = 10\ \text{nm}, \ E = 0.1422\ eV, m^* = 0.067\ m_e\), inspired in semiconductor quantum structures. Our choice of parameters guarantees that most momentum components of the initial state tunnel through the potential. Figure 1 shows a plot of \(|\psi(L, \tau)|^2\), calculated at the barrier edge \(x = L\) as a function of time in units of the free passage time \(\tau_f = mL/(\hbar k) = 11.56\ \text{fs}\). We have used Eq. (3), though Eq. (3) holds the same. The time-dependent solution is normalized by \(|T(k)|^2 = 5.332 \times 10^{-9}\). One sees that as soon as \(\tau \neq 0\) the probability density starts to grow up. As discussed elsewhere [20], this is due to the non-relativistic character of the description. Einstein causality may be fulfilled by cutting off the contributions to the probability density smaller than \(\tau_0 = L/c\). In our example \(\tau_0 = 0.033\ \text{fs}\) or \(\tau_0/\tau_f = 0.0028\), too small to be appreciated in Fig. 1. At early times one sees a time domain resonance structure. Thereafter the probability density approaches essentially its asymptotic value. We found that the resonant sum is the relevant contribution to the time domain resonance since that of the free-type term is quite small and varies smoothly with time. In the transmitted region, \(x > L\), not shown here, the time domain resonance becomes a propagating structure, as follows from Eq. (3). The time domain resonance corresponds to a transient effect and as it propagates through the transmitted region becomes smaller and smaller. Asymptotically, at large distances and times, it becomes very small while the free-type term becomes the dominant contribution with its wavefront propagating with velocity \(v = \hbar k/m\). Calculations using the absorbing initial condition exhibit a similar time domain resonance. Hence a linear combination of reflecting and absorbing initial conditions should also exhibit it.

The time domain resonance represents a distribution of traversal times. The corresponding peak represents the largest probability to find the tunneling particle at the barrier edge \(x = L\). In our example, as shown in Fig. 1, the time domain resonance peaks at \(\tau_p = 5.326\ \text{fs}\), faster than the free passage time across the same distance of \(10\ \text{nm}\), that is, \(\tau_p/\tau_f = 0.46\). Note that the distribution is quite asymmetric. Although the first resonance term of the solution provides the main contribution, convergence of the series usually requires to sum up to 100 terms. The inset displays the probability density from \(\tau/\tau_f = 2\) up to \(\tau/\tau_f = 20\). One sees a small structure around \(\tau/\tau_f = 3\) and then the probability density decreases very fast towards unity, the stationary regime. The main range of traversal times occurs around the peak value \(\tau_p\). We define the width of the distribution, \(\Delta \tau\), by the rule of the half-width at half-maximum. This yields \(\Delta \tau = 13.48\ \text{fs}\) or \(\Delta \tau/\tau_f = 1.16\). The resonance is broad, since \(\Delta \tau \approx 2\tau_p\). We have found that for fixed \(V_0\) and \(E\), and a decreasing \(L\), the width diminishes. The same occurs for fixed \(E\) and \(L\), and an increasing \(V_0\). Systematically, however, \(\Delta \tau > \tau_p\). For the sake of comparison, the arrows in Fig. 2 indicate the values calculated for a number of definitions of tunneling times existing in the literature for the rectangular barrier potential [22], as the Larmor time of Bâz and Rybchenko, \(\tau_{LM}\); the semiclassical or Böttiker-Landauer time, \(\tau_{BL}\); the Böttiker traversal time, \(\tau_B\), and the phase-delay time, \(\tau_D\) [23]. All of them fall within the broad range of values given by \(\Delta \tau\). Note, however, that the Böttiker traversal time \(\tau_B\) is the closest to \(\tau_p\). As shown below we have found this situation extensively in our numerical calculations. Also, since the barrier is opaque, \(\tau_B\) is close to \(\tau_{BL}\).

We refer briefly to approaches to the tunneling time problem based on the Feynman path integral method [3,4,5]. For plane waves and a rectangular barrier potential Fertig [7] has derived an expression, \(C(\tau)\), that gives the probability amplitude that a particle remains a time \(\tau\) in a region, (Eq. (3) of Ref. [8]). Recently Yamada [8] has plotted \(G(\tau) = |C(\tau)|^2\) versus \(\tau\) (Fig. 2 of Ref. [8]). His parameters are the same as in our Fig. 1, i.e., \(V_0/E = 5\) and \(kL = 5\). Our calculation for \(|\psi(L, \tau)|^2\) resembles the average shape of \(G(\tau)\), provided its noisy behavior is ignored. Note, however, that the meaning of both quantities is different. As indicated by Yamada, \(G(\tau)\) refers to a ‘residence time’ [24] whereas our approach corresponds to a ‘passage’ or traversal time [23].

In Fig. 2 we plot \(\tau_p\) (solid squares) for different values of the opacity \(\alpha = k_0L\), with \(k_0 = [2mV_0]^{1/2}/\hbar\). Keeping \(V_0\) fixed and varying \(L\) defines \(\alpha(L)\). We can then identify two regimes, one in the range \(2 \leq \alpha(L) \leq 5\), the tunneling regime, where \(\tau_p\) remains almost constant as \(\alpha(L)\) increases, and another regime, the opaque regime, with \(\alpha(L) > 5\), where we find that \(\tau_p\) increases linearly. The first behaviour above is related to the first top-barrier S-matrix pole and the second one to the components of the incident wave that go above the barrier. There is still another regime, not shown in Fig. 2 where \(\alpha(L) < 1\), that corresponds to very shallow or very thin barriers or both and will not be considered here. There the free-type terms in Eq. (3) dominate over the resonant contribution. For comparison we plot the Böttiker traversal time \(\tau_{BL}\) (hollow circles). We see that \(\tau_{BL}\) remains rather close to \(\tau_p\). Note, however, that \(\tau_{BL}\) behaves linearly in the whole range. This different qualitative behaviour as a function of \(L\) between both times deserves further study.

The inset in Fig. 2 exhibits a similar comparison for the opacity \(\alpha(V_0)\), with \(L\) fixed and varying \(V_0\). Here we observe that \(\tau_B\) remains quite close to \(\tau_p\) in the whole range. Regarding the phase-delay time \(\tau_D\), its predic-
tions usually fall within the width $\Delta \tau$. For fixed $V_0$ and $E$, $\tau_D$ as a function of $L$ exhibits qualitatively a different behaviour than that of Fig. 1 (See Fig. 5 in ref. [4]).

To end we stress that the largest probability to find the tunneling particle at the barrier width, given by $\tau_p$, is sensitive to both variations of the barrier width $L$ and of the height $V_0$, and also, that the Büttiker traversal time is found very close to the value of $\tau_p$ though we find qualitative differences between them as a function of $L$.

G. G-C. thanks M. Moshinsky for useful discussions and acknowledges support of DGAPA-UNAM under grant IN116398. We also acknowledge partial financial support of Conacyt under contract no. 431100-5-32082E.

[1] E. E. Mendez, in Physics and Applications of Quantum Wells and Superlattices, edited by E. E. Mendez and K. Von Klitzing (Plenum, New York, 1987) p. 159.
[2] M. F. Crommie, C. P. Lutz, and D. M. Eigler, Science 262, 218 (1993).
[3] E. H. Hauge and J. A. Stovneng, Rev. Mod. Phys 61, 917 (1989); R. Landauer and Th. Martin, ibid. 66, 217 (1994).
[4] T. E. Hartman, J. Appl. Phys. 33, 3427 (1964).
[5] F. Smith, Phys. Rev. 118, 349 (1960).
[6] See for example: D. Sokolovski, S. Brouard, and J. N. L. Connor, Phys. Rev. A 50, 1240 (1994).
[7] H. A Fertig, Phys. Rev. Lett. 65, 2321 (1990); Phys. Rev. B 47, 1346 (1993).
[8] N. Yamada, Phys. Rev. Lett. 83, 3350 (1999).
[9] S. Collins, D. Lowe, and J. R. Barker, J. Phys. C 20, 6213 (1987).
[10] V. Delgado and J. G. Muga, Ann. Phys. (N.Y) 248, 122 (1996).
[11] M. Moshinsky, Phys. Rev. 88, 625 (1952).
[12] K. W. H. Stevens. J. Phys. C 16, 3649 (1983).
[13] P. Moretti, Phys. Rev. A 46, 1233 (1992).
[14] S. Brouard and J. G. Muga, Phys. Rev. A 54, 3055 (1996).
[15] For the rectangular barrier, an expression analogous to Eq. (3) may be derived without using resonant states, G. García-Calderón, J. L. Mateos and M. Moshinsky (unpublished).
[16] G. García-Calderón and A. Rubio, Phys. Rev. A 55, 3361 (1997).
[17] P. Szriftgiser, D. Guéry-Odelin, M. Arndt, and J. Dalibard, Phys. Rev. Lett. 77, 4 (1996); Th. Hils, J. Felber, R. Gähler, W. Gläser, R. Golub, K. Habicht, and P. Wille, Phys. Rev. A 58, 4784 (1998).
[18] R. Gähler and R. Golub, Z. Phys. B 56, 5 (1984).
[19] G. García-Calderón and R. E. Peierls, Nucl. Phys. A 265, 443 (1976).
[20] G. García-Calderón, A. Rubio and J. Villavicencio, Phys. Rev. A 59, 1758 (1999).
[21] H. M. Nussenzveig, Nucl. Phys. 11, 499 (1957).
[22] M. Büttiker, Phys. Rev. B 27, 6178 (1983).

See, respectively, Eqs. (1.4), (1.7), (3.12) and (3.2) of Ref. [2].

The ‘residence time’ involves the integral of the probability density along the internal region of the interaction. This definition does not distinguish whether particles are finally transmitted or reflected and hence it is not appropriate to describe traversal times.

FIG. 1. Plot of $|\psi(L, \tau)|^2$ at the barrier edge $x = L = 10 \, \text{nm}$ as a function of time in units of the free passage time $\tau_f$. The inset shows $|\psi(L, \tau)|^2$ at larger times. The arrows indicate the values of the Larmor time $\tau_{LM}$, the semi-classical time $\tau_{BL}$, the Büttiker traversal time $\tau_B$, and the phase-delay time $\tau_{D}$. See text.

FIG. 2. Plot of the exact time domain resonance peak $\tau_p$ (solid squares) versus the opacity $\alpha(L)$ ($V_0$ fixed). For comparison we plot the Büttiker traversal time $\tau_B$ (hollow circles). The inset shows a similar calculation versus the opacity $\alpha(V_0)$ ($L$ fixed). See text.
FIG. 2

Tau (fs) vs. \( \alpha (L) \) and \( \alpha (V_0) \).

Inset: \( \alpha (V_0) \) vs. \( \alpha (L) \).