Quantum shutter approach to tunneling time scales with wave packets

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(Dated: December 2, 2018)

The quantum shutter approach to tunneling time scales (G. García-Calderón and A. Rubio, Phys. Rev. A 55, 3361 (1997)), which uses a cutoff plane wave as the initial condition, is extended in such a way that a certain type of wave packet can be used as the initial condition. An analytical expression for the time evolved wave function is derived. The time-domain resonance, the peaked structure of the probability density (as the function of time) at the exit of the barrier, originally found with the cutoff plane wave initial condition, is studied with the wave packet initial conditions. It is found that the time-domain resonance is not very sensitive to the width of the packet when the transmission process is in the tunneling regime.

PACS numbers: 03.65.Xp, 03.65.Ca, 03.65.Ta

I. INTRODUCTION

Tunneling is one of the most important quantum phenomena that has been widely applied in science and technology. For years, the stationary treatments of tunneling were sufficient for many practical purposes, and the details of tunneling dynamics were not urgent issues to investigate. This is not the case anymore. The interest in tunneling dynamics is increasing as, for example, the number of carriers involved in tunneling events decreases due to the rapid downsizing of semiconductor devices. In principle, the tunneling dynamics can be completely understood if one can solve the time dependent Schrödinger equation, taking other degrees of freedom into account that affect the tunneling particles. This is, however, a difficult task in general. It is thus important to study the time scales of tunneling dynamics (tunneling times) in simplified models and use them for qualitative understanding of the tunneling dynamics in realistic systems. There are many approaches to define or measure the tunneling times in simplified models 1–4, and the quantum shutter approach 5 is one of them. The present paper concerns a generalization of the quantum shutter approach.

Let us consider a one dimensional scattering problem where a particle is incident on a potential $V(x)$. The time scales that characterize the tunneling dynamics are “embedded” in the wave function. To extract them from the wave function, the quantum shutter approach 5 uses a cutoff plane wave as the initial condition and monitors how the probability density changes in time at a specified position (e.g., at the exit of the barrier) or in a spatial region (e.g., in the well region in a double barrier structure) to find out the time scales that characterize the transient behavior of the wave function (from non-stationary to stationary). The use of a cutoff plane wave initial condition can be understood as an analogy to the use of a step input in the study of the temporal response of an electrical (e.g., RCL) circuit.

Studies of tunneling dynamics involving cutoff plane waves go back back to Stevens 6, who argued the signal velocity under the barrier by applying the contour deformation technique developed by Brillouin 7. This technique allows one to decompose a wave propagating in a dispersive medium into three parts: the fore-runners, the monochromatic part oscillating with the same frequency as the source, and the after-runners; the signal velocity is then defined as the velocity with which the monochromatic front moves. The under-the-barrier signal velocity found by Stevens was, however, questioned later by Teranishi et al 8, Jauho and Jonson 9, and Ranfagni et al 10; these authors showed that the monochromatic front to which the signal velocity is attributed is in fact not appreciable in magnitude. Through these works, it was recognized that it is not appropriate to focus only on the monochromatic part of the wave. Büttiker and Thomas 11 and Muga and Büttiker 12 thus studied not only the monochromatic part but also the fore-runners in detail, whereas Brouard and Muga 13 turned their attention to the total wave function (under a cutoff plane wave initial condition) and studied its properties with an exact analytical expression for the wave function which they derived. Independently, García-Calderón and Rubio 14 derived an exact analytical expression for the wave function with a cutoff plane wave initial condition and applied it to the analysis of the transient behaviors in the tunneling dynamics. It may be said that these studies formed a new area of research in the field of quantum...
dynamics, where one explores the tunneling dynamics, especially its transient behaviors, by using exact analytical expressions for the wave functions with cutoff plane wave initial conditions. The quantum shutter approach and the approach by Brouard and Muga use the same tool called M function [see Eq. 3] to express the wave functions in analytical manners. They differ, however, in the following respect: in addition to the $M$ function, the quantum shutter approach uses the resonant eigenfunctions, while the approach by Brouard and Muga uses an entire function that arises from a pole expansion of a function involved in the momentum eigenfunction expansion of the wave functions. In [14], an analytical expression for the transmitted wave was obtained in sole terms of the $M$ function and the poles and the residues of the transmission amplitude. Another interesting and unexpected aspect of the quantum shutter approach is that it has a close relationship with the consistent history approach to the tunneling time problem as shown in [14]. In particular, the probability density at the exit of a rectangular barrier under a cutoff plane wave initial condition, a quantity of major concern in the quantum shutter approach, coincides, when properly normalized, with a function $G_p(t)$ that is defined in the consistent history approach. Function $G_p(t)$ allows us to associate the transient behaviors of the wave function with the interference between Feynman histories with different tunneling times, which provides a novel viewpoint to the transient behavior. In this way, the quantum shutter approach is related not only to the stream of research that began with the work of Stevens but also to a relatively new approach, the consistent history approach, to the tunneling time problem. In Ref. [13], the consistent history approach was used to give different tunneling times in a unified manner.

The quantum shutter approach, formulated for a general (but finite-range) potential $V(x)$ [in this paper $V(x)$ is such that it vanishes for $x < 0$ and for $x > d$] and uses, for example, the following form of the cut off plane wave as the initial wave function:

$$
\Psi(x, 0) = \begin{cases} 
2i \sin k_0 x & \text{for } x < 0 \\
0 & \text{for } x \geq 0,
\end{cases}
$$

(1)

where $k_0$ is the wave number. This setup corresponds to the physical situation where a beam of particles with energy $E_0 = \hbar^2 k_0^2 / 2m$ (though not exactly monochromatic due to the sharp front of the wave) impinges on a shutter placed at $x = 0$, just at the left edge of the potential; the tunneling process begins with the instantaneous opening of the shutter at $t = 0$, enabling the incoming wave to interact with the potential for $t > 0$. When the initial condition is given by Eq. (1), the exact solution of the time dependent Schrödinger equation along the transmitted region $x \geq d$ is found to be [14, 16]

$$
\Psi(x, t) = T(k_0) M(x, k_0; t) - T(-k_0) M(x, -k_0; t)
$$

(2)

where $k_n$ is the $n$-th pole of the transmission amplitude $T$ (poles lie in the lower-half of the complex $k$ plane), $r_n$ is the associated residue, and the $M$ functions are defined by

$$
M(x, q; t) = \frac{i}{2\pi} \int_{-\infty}^{\infty} dk \frac{e^{ikx - \bar{q}k^2 t / 2m}}{k - q}
$$

(3)

$$
= \frac{1}{2} e^{(imx^2 / 2ht)} w(iy_q),
$$

(4)

where $q = k_n \pm \bar{k}_0$; the function $w(z)$, which is often called Faddeeva function, is related to the complex complementary error function as $w(z) = e^{-z^2} \text{erfc}(-iz)$ [20], and $y_q$ is given by

$$
y_q = e^{-i\pi / 4} \sqrt{\frac{m}{2\bar{q}t}} \left[ x - \frac{\bar{q}q}{m} \right].
$$

(5)

The $w$ function appears in many fields of physics and mathematics, so that it has been well studied and its
properties have been well understood \[21\]. Some computer programs are available for numerical calculation of the \( w \) function \[22\].

Let us now consider the following initial condition:

\[
\Psi(x, 0) = A \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} \left( e^{ikx} \right), \tag{6}
\]

where \( A = \sqrt{\Delta \left\{ 1 + (\Delta/k_0)^2 \right\}} / 2\pi \) with \( \Delta > 0 \), and “c.c.” stands for complex conjugate. An important feature of this \( \Psi(x, 0) \) is that it automatically vanishes for \( x > 0 \). This is immediately seen from the fact that the integrand \( e^{ikx} \) vanishes automatically for \( x < 0 \), due to the Lorentzian momentum distributions. Equation (6) thus leads us to a natural setup of the shutter problem with a normalized wave initial condition. Equation (8) follows directly from the eigenfunction expression (9). Substituting Eq. (6) into Eq. (9), we have

\[
\Psi(x, t) = \left\{ \begin{array}{ll}
4\pi A e^{\Delta x} \sin k_0 x & \text{for } x < 0 \\
0 & \text{for } x \geq 0.
\end{array} \right. \tag{7}
\]

This represents a wave packet. A measure of the packet width is \( 1/\Delta \). We can easily prove that the wave packet is normalized, i.e., \( \int dx |\Psi(x, 0)|^2 = 1 \). If the above \( \Psi(x, 0) \) is multiplied by a constant \( i/\sqrt{\Delta} \) and the limit \( \Delta \to 0 \) is taken, Eq. (1) is reproduced. The above \( \Psi(x, 0) \) is therefore a wave packet counterpart of the cut-off plane wave initial condition. Equation (10) thus leads us to a natural setup of the shutter problem with a normalized wave packet initial condition which vanishes automatically for \( x > 0 \) due to the Lorentzian momentum distributions.

Let us derive an analytical expression for \( \Psi(x, t) \) under the initial condition given by Eq. (11). For definiteness, we shall limit our attention to the analytical expression only in the transmitted region \( x > d \). We start from the following expression for the time evolved wave function for the transmitted region:

\[
\Psi(x, t) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} \phi(k) T(k) e^{ikx - i\hbar k^2 t/2m}, \tag{8}
\]

where \( \phi(k) \) is the \( k \)-space wave function (i.e., the Fourier transform of the initial wave function) defined by

\[
\phi(k) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-ikx} \Psi(x, 0). \tag{9}
\]

Equation (8) follows directly from the eigenfunction expansion of the wave function in the transmitted region. Substituting Eq. (9) into Eq. (8), we have

\[
\phi(k) = \sqrt{2\pi} A \left( \frac{1}{k - k_0 + i\Delta} - \frac{1}{k + k_0 + i\Delta} \right). \tag{10}
\]

Next, we expand the transmission amplitude in terms of its complex poles and the corresponding residues by using a special form of the Mittag-Leffler theorem due to Cauchy \[23\]. It may be expanded as \[14\] 24

\[
T(k) = \sum_{n=-\infty}^{\infty} \left( \frac{r_n}{k - k_n} + \frac{r_n}{k_n} \right). \tag{11}
\]

The substitution of Eqs. (10) and (11) into the right-hand side of Eq. (8) yields the following quantity:

\[
\left( \frac{1}{k - k_0 + i\Delta} - \frac{1}{k + k_0 + i\Delta} \right) \left( \frac{1}{k - k_n} + \frac{1}{k_n} \right),
\]

which, upon expansion, gives four terms. To two of the four terms, we apply the partial fraction expansion

\[
\frac{1}{k \pm k_0 + i\Delta} \left( \frac{1}{k - k_n} - \frac{1}{k \pm k_0 + i\Delta} \right) \tag{12}
\]

and express the resultant \( k \) integrals in terms of \( M \) functions. We then have

\[
\Psi(x, t) = -2\pi i A
\times \sum_n \left( \frac{r_n}{k_0 - k_n} + \frac{r_n}{k_n} \right) M(x, k_0 - i\Delta; t)
- \sum_n \left( \frac{r_n}{-k_0 - k_n} + \frac{r_n}{k_n} \right) M(x, -k_0 - i\Delta; t)
- \sum_n \left( \frac{r_n}{k_0 + k_n + i\Delta} + \frac{r_n}{k_0 - k_n - i\Delta} \right) M(x, k_n; t) \right]. \tag{13}
\]

Due to Eq. (11), the first and the second sums over \( n \) in the square brackets in Eq. (13) give \( T(k_0 - i\Delta) \) and \( T(-k_0 - i\Delta) \), respectively. We thus arrive at

\[
\Psi(x, t) = -i\sqrt{\Delta \left\{ 1 + (\Delta/k_0)^2 \right\}}
\times \left[ T(k_0 - i\Delta) M(x, k_0 - i\Delta; t)
- T(-k_0 - i\Delta) M(x, -k_0 - i\Delta; t)
- 2k_0 \sum_n \frac{r_n}{k_0^2 - (k_0 + i\Delta)^2} M(x, k_n; t) \right]. \tag{14}
\]

This is the analytical expression for the time evolved wave function in the transmitted region under the initial condition given by Eq. (7). The analytical solution under the cutoff plane wave initial condition, Eq. (2), can be correctly reproduced from Eq. (14) if we multiply Eq. (14) by a constant \( i/\sqrt{\Delta} \) and then take the limit \( \Delta \to 0 \). It is also possible to derive an analytical expression for \( \Psi(x, t) \) in terms of \( M \) functions in other regions of space, although we concentrate on the transmitted region.

To use Eq. (14), we have to find the poles \( \{k_n\} \) and calculate the residues \( \{r_n\} \) and the \( w \) functions numerically. The residues may be calculated in general by using the simple relationship

\[
r_n = iu_n(0) u_n(d) e^{-ik_n d}, \tag{15}
\]

where \( u_n \) is the \( n \)-th spherical Bessel function of the first kind.
where, as discussed in the appendix A of Ref. [3], the resonant eigenfunctions $u_n(x)$ are solutions to the time-independent Schrödinger equation

$$\frac{d^2 u_n(x)}{dx^2} + \left[ k_n^2 - \frac{2m}{\hbar^2} V(x) \right] u_n(x) = 0$$  \hspace{1cm} (16)

satisfying the outgoing boundary conditions,

$$\left. \frac{d}{dx} u_n(x) \right|_{x=0} = -i k_n u_n(0); \quad \left. \frac{d}{dx} u_n(x) \right|_{x=d} = i k_n u_n(d),$$

and the normalization condition,

$$\int_0^d u_n^2(x) dx + \frac{u_n^2(0) + u_n^2(d)}{2k_n} = 1.$$  \hspace{1cm} (18)

For a rectangular potential of height $V_0$ and width $d$, the resonant eigenfunctions read,

$$u_n(x) = C_n e^{i q_n x} + D_n e^{-i q_n x} \quad (0 \leq x \leq d)$$  \hspace{1cm} (19)

where $q_n = \sqrt{k_n^2 - k_V^2}$, $k_V = \sqrt{2mV_0/\hbar}$, $D_n = (q_n + k_n)/(q_n - k_n)$ and $C_n$ may be obtained from the normalization condition given above. Alternatively, one may use the following explicit relationship between $k_n$ and $r_n$ to calculate $r_n$:

$$r_n = \frac{4k_n^2(k_n^2 - k_V^2)^{3/2} e^{-ik_n d}}{k_V^2(k_n^2 + 2i) \sin(d\sqrt{k_n^2 - k_V^2})}.$$  \hspace{1cm} (20)

One can derive Eq. (20) directly from $r_n = \exp(-ik_n d)/g'(k_n)$, where the prime stands for $d/d k$ and $g(k) = \exp(-ik d)/T(k)$; the exact analytical expression for the transmission amplitude $T(k)$ is available in the standard textbooks of quantum mechanics.

Readers might have noticed that both Eqs. (11) and (17) correspond to an initially vanishing probability current density, i.e., $J(x,0) = 0$. This is, however, not a general feature of the quantum shutter approach. The approach can be formulated even if $\Psi(x,0) = 2i \sin k_0 x = e^{ik_0 x} - e^{-ik_0 x}$ in Eq. (11) is replaced by $\Psi(x,0) = ae^{ik_0 x} + be^{-ik_0 x}$ with arbitrary constants $a$ and $b$. For this general plane wave initial condition, $J(x,0) \neq 0$ in general. In the same vein as above, we can construct a wave packet counterpart, for which $J(x,0) \neq 0$ as well. For this wave packet initial condition with nonzero flux, one may also obtain an analytical expression for the time evolved wave function in terms of $M$ functions.

**III. EXAMPLE**

In the rest of this paper, we apply Eq. (14) to tunneling through a rectangular barrier to study how the time-domain resonance [16] depends on the width of the incident packets. Assuming a rectangular barrier of height $V_0 = 0.3$ eV that extends from $x = 0$ to $x = 4$ nm, we have calculated the probability density at the exit of the barrier, $|\Psi(d,t)|^2$, for a particle of effective mass $m = 0.067m_e$ ($m_e$ being the bare electron mass) with (central) energy $E_0 = \hbar^2 k_0^2/2m = 0.01$ eV ($k_0 \approx 0.133$ nm$^{-1}$). The above refers to typical semiconductor heterostructure parameters [16]. Figure 1 shows the results for different values of $\Delta$, where the time axis is in units of the free passage time $t_f = md/\hbar k_0 \approx 17.5$

![FIG. 1: Plot of $|\Psi(d,t)|^2$ at the barrier edge $x = d = 4$ nm as the function of time in units of the free passage time $t_f$. The initial condition is given by Eq. (11) in (a) and by Eq. (7) in (b) and (c). We calculated numerically 1000 poles in the 3rd quadrant and also in the 4th quadrant in the complex $k$ plane, and used them with Eqs. (8) and (13) to plot these graphs.](image-url)
s. Figure 1(a) shows the plot of $|\Psi(d, t)|^2$ for the case of $\Delta = 0$ calculated from Eq. (2); we can see a transient behavior of the probability density that starts from zero, increases to the maximum, and then approaches its asymptotic value $|T(k_0)|^2$ as shown in the inset of Fig. 1(a). The peaked structure is an example of the time-domain resonance. In the present example, the time $t_p$ that gives the maximum of $|\Psi(d, t)|^2$ is about 0.303$\tau$. Figures 1(b) and (c) obtained from Eq. (14) show reasymptotic value zero, increases to the maximum, and then approaches its peak value of $\Delta/k_0 = 0.75 (\Delta \approx 0.10 \text{ nm}^{-1})$ and the case of $\Delta/k_0 = 4.0 (\Delta \approx 0.53 \text{ nm}^{-1})$. Unlike the case of Fig. 1(a), the probability density approaches zero for large values of $t$ in Figs. 1(b) and (c). This is simply because the particle is eventually reflected or transmitted for the wave packet initial condition.

We first find from the graphs that the peaked nature of $|\Psi(d, t)|^2$ is not lost (i.e., the time-domain resonance is preserved) even for relatively large values of $\Delta$ (and thus for relatively narrow packets in configuration space). In the case of Fig. 1(b), the packet width $1/\Delta$ is more than twice the barrier width. In the case of Fig. 1(c), where the time domain resonance is still clear, the packet width is less than half of the barrier width.

Secondly, we find that $t_p$ does not depend significantly on the value of $\Delta$ in the tunneling regime. In the case of Fig. 1(b), where the average energy of the particle, $\langle E \rangle = \{1 + (\Delta/k_0)^2\} E_0$, is approximately 0.016 eV, we have $t_p/t_0 \approx 0.288$, so that the shift of $t_p/t_0$ from the case of Fig. 1(a) is only about 5%. In the case of Fig. 1(c), where $\langle E \rangle \approx 0.17$ eV, we have $t_p/t_0 \approx 0.221$, which shows as much as 27% shift from the case of Fig. 1(a). Although the average energy is below the barrier height in both cases, we must note that only the case of Fig. 1(b) can be associated with tunneling as explained below.

In what follows we refer to two different approaches to distinguish between tunneling and non-tunneling processes. The first one involves a stationary analysis whereas the second one deals with a time-dependent description. For wave packet initial conditions, the first approach relies on the computation of both the tunneling probability $P_{\text{under}}$ (i.e., the probability of under-the-barrier transmission), and the non-tunneling probability $P_{\text{over}}$ (i.e., the probability of over-the-barrier transmission) defined by

$$P_{\text{under}} = \int_{0}^{k_0} dk |T(k)|^2 |\phi(k)|^2, \quad (21)$$

$$P_{\text{over}} = \int_{k_0}^{\infty} dk |T(k)|^2 |\phi(k)|^2. \quad (22)$$

In the case of Fig. 1(b), $P_{\text{under}} \approx 0.00161$ and $P_{\text{over}} \approx 0.00117$, so we affirm that under-the-barrier transmission slightly dominates, and in this sense, the transmission is in the tunneling regime. In the case of Fig. 1(c), $P_{\text{under}} \approx 0.0111$ and $P_{\text{over}} \approx 0.0426$, so that over-the-barrier transmission dominates and the process is not in the tunneling regime. The second approach deals with a time-frequency analysis, where we introduce the local average frequency $\omega_{av}$ (the instantaneous frequency of the wave function) and the instantaneous bandwidth $\sigma$ (the spread of frequencies around $\omega_{av}$) as follows:

$$\omega_{av}(t) = -\text{Im} \left( \frac{1}{\Psi} \frac{\partial \Psi}{\partial t} \right), \quad (23)$$

$$\sigma(t) = \left| \text{Re} \left( \frac{1}{\Psi} \frac{\partial \Psi}{\partial t} \right) \right|. \quad (24)$$

The local average frequency was used in Refs. 12, 18 and the local bandwidth in Ref. 18 in the studies of tunneling time. It is immediate from Eq. (21) that $\sigma = 0$, i.e., the wave function has a single instantaneous frequency, when $\partial |\Psi(x, t)|^2/\partial t = 0$, which holds at the time domain resonance peak at $t = t_p$. Therefore, the time domain resonance peak is characterized by a single instantaneous frequency $\omega_{av}$, or equivalently, by a single energy $h\omega_{av}$. This was exemplified in Ref. 18.

We have calculated $\omega_{av}$ at the time domain resonance peak, namely, $\omega_{av}(t = t_p)$, to find that $\omega_{av}/\omega_0$, with $\omega_0^2 = V_0/h$, is $\approx 0.792, 0.944,$ and $1.583$ for the case of Fig. 1(a), (b), and (c), respectively. This implies that the time domain resonance peak is associated with tunneling for the case of Figs. 1(a) and (b), but it is not for the case of Fig. 1(c) since $\omega_{av}/\omega_0 > 1$. We have thus shown, using two different approaches, that Figs. 1(a) and (b) correspond to tunneling, but Fig. 1(c) does not.

As shown above, $t_p$ is not very sensitive to the width of the packets in the tunneling regime. This in turn justifies the use of the cutoff plane wave initial condition as far as the estimation of the value of $t_p$ in the tunneling regime is concerned; $t_p$ is expected to characterize the earliest tunneling response of the system and thus, it would be of relevance for device applications. A comparison of $t_p$ with other tunneling time scales, such as the delay time, the B"{u}ttiker traversal time, and the semiclassical time, has been given elsewhere.

In Ref. 16, the time-domain resonance was also studied with a cutoff pulse initial condition given by $\Psi(x, t) = 2i \sin k_0 x$ for $-a \leq x \leq 0$, and zero otherwise. It was found that the resulting time-domain resonance structure is almost identical to the one obtained with the semi-infinite cutoff plane wave initial condition, i.e., Eq. (11). This is consistent with our result that the time-domain resonance structure is not quite sensitive to the packet width. On the other hand, the oscillatory behavior of the probability density in the “post resonance” time domain (see Fig. 7 in Ref. 12) cannot be seen in our results. This implies that the probability density in the “post resonance” time domain is sensitive to the shape of the incident wave.
IV. SUMMARY

In summary, we have extended the type of initial conditions used in the quantum shutter approach from shuttered plane waves to a certain class of wave packets. This makes it possible to study the “size effect” of the packets on the various results that had been obtained from the quantum shutter approach with shuttered plane wave initial conditions. We have derived an analytical expression for the time evolved wave function, Eq. (14), under the wave packet initial condition given by Eq. (7). Focusing on the size effect on the time domain resonance, we exemplified that (i) the time-domain resonance structure is present even when the packet width $\frac{1}{\Delta}$ is much shorter than the barrier width, a situation that is quite different from those considered in the original quantum shutter approach, where the incident wave is semi infinite, and (ii) the time $t_p$ at which the time resonance peak occurs is not very sensitive to the packet width when the transmission process is in the tunneling regime. In this sense, the time domain resonance is robust against the change of the initial conditions.

V. ACKNOWLEDGMENTS

N.Y. thanks the Department of Physics, UNAM for their hospitality. He thanks H. Yamamoto for encouragement. N.Y. carried out a part of his numerical calculations on SX7 at the Information Synergy Center, Tohoku University. G.G-C and J.V acknowledge partial financial support of DGAPA-UNAM under grant No. IN108003.

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