A New Time-Scale for Tunneling

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We study the tunneling through an oscillating delta barrier. Using time periodicity of the model, the time-dependent Schrödinger equation is reduced to a simple but infinite matrix equation. Employing Toeplitz matrix methods, the infinite matrix is replaced by a 3×3 matrix, allowing an analytical solution. Looking at the frequency dependence of the transmission amplitudes, one observes a new time scale which dominates the tunneling dynamics. This time scale differs from the one previously introduced by Büttiker and Landauer. The relation between these two is discussed.

1. INTRODUCTION

The question regarding the actual time spent during tunneling through a barrier has been in discussion for over half a century.⁽¹⁻⁶⁾ The introduction of high-speed tunneling-based semiconductor devices in recent years⁽⁷⁾ has brought new urgency to the problem. However, in spite of the long history of this subject, it still remains controversial.

Most of the opinions on this matter can be classified into three categories. The most apparent way to define and calculate tunneling times is through the dynamics of the wave packet. Some suggestions use the stationary phase approximation and obtained the time the peak of the wave packet spent in the barrier region.⁽²⁾ In a more recent version of this approach, the peak is replaced by the centroid of the packet.⁽⁸⁾ Nevertheless, this approach is problematic. It has been shown⁽⁹⁾ by an explicit example that a tunneling situation can be set up such that the peak or centroid of the transmitted packet emerges before the peak or centroid of the incident packet has even arrived at the barrier, leading to negative time and demonstrating the lack of causal relationship.

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A more sophisticated way involves the introduction of a physical clock which is used to determine the time elapsed during tunneling. One can look at either the effect of the clock on the tunneling particle or at the clock variable itself. Mainly, three versions of clocks have been proposed and investigated in the literature. The first clock approach studies the precession of the spin of the tunneling particle due to a uniform infinitesimal magnetic field confined to the barrier region.⁽¹⁰⁾ It was later noted that in addition to the precession in the plane perpendicular to the magnetic field, the spin-up component in the magnetic field direction tunnels preferentially due to the Zeeman splitting.⁽¹¹⁾ These two processes caused by the field can be used as physical clocks. One gets two different time scales from these two. The two time scales are equal to the real and imaginary parts of the complex time obtained using the Feynman approach.⁽¹²⁾ A second clock approach uses an incident wave composed of two interfering waves.⁽¹³⁾ If these two are of opposite spin direction, the total incident particle flux is uniform in time with an oscillatory spin.

Büttiker and Landauer (BL) studied tunneling through a rectangular barrier with a small oscillating component added to the height.⁽³⁾ The incident particles with energy E can absorb or emit modulation quanta $\hbar\Omega$ during tunneling, leading to the appearance of sidebands with energies $E \pm n\hbar\Omega$ and corresponding intensities $I_{\pm n}$. Looking at the Ω dependence of these quantities, BL determined the critical frequency as that in which the transition between the behavior at the two limits of quasi-static barrier and the average barrier occurs. The inverse of this frequency is an indication of the time scale of the tunneling process.

Third, there are many who object to the question in the first place.⁽¹⁴⁾ It is often said that the concept of tunneling time is not well defined in the context of quantum mechanics, and does not correspond to any observable. This is related to the absence of a time operator in quantum mechanics. This problem can be bypassed using an operator which measures whether the particle is in the barrier or not, and then (in time-dependent problems) averaging over time. The result, divided by the incident flux, is termed the "dwell time."⁽¹¹⁾ Nevertheless, this solution is far from being satisfactory, since taking expectation values, one cannot distinguish between the transmitted and reflected particles, and thus the time obtained is just an average over two (possibly different) times related to these two processes. This problem follows from the absence of a well-defined history of a quantum particle.⁽¹⁵⁾ As far as the particle was not measured in the barrier, it was not there at all and thus formally the time spent in the barrier is zero.⁽¹⁶⁾

In this paper we do not want to take a stand in this debate, but rather to point out that even if one argues that the *actual* time spent inside the barrier region is not defined or zero, it is agreed that the *wave function* spent a finite time inside the barrier. The question about the time scales related to the wave function transition through the barrier is at least as important as the (maybe more fundamental) former one. After all, the quantum dynamics is determined by the wave function, and thus many questions in which time scales are relevant are really not related to the *actual* time as measured experimentally, but rather to the time in which the wave packet—describing the particle in times it is *not measured*—was in the regime in interest. This approach is motivated by the physical clocks approach. Again, even if the application of the proposed experiments to the "strong" question of tunneling time is arguable, one cannot deny the need for tunneling time scales while considering the process in a time-dependent environment such as considered in the BL approach. In what follows we use the same approach and consider the tunneling process through an oscillating delta barrier

$$V(x, t) = V_0 \,\delta(x)(1 + \varepsilon \cos(\Omega t)) \tag{1}$$

As in the BL case, the tunneling particle can absorb or emit any number of energy quanta $h\Omega$ while being transmitted or reflected (see Fig. 1). Using the time periodicity of the Hamiltonian, the Schrödinger equation is reduced to the inversion of an infinite tridiagonal matrix. In practice, the matrix can be truncated very efficiently and reliable numerical solutions are easily obtained. In the large quantum numbers regime the three-diagonals elements become almost constant, and the matrix is approximately a



Fig. 1. Oscillating delta function barrier.

Toeplitz matrix.^(17, 18) In this case one can reduce the problem to the-inversion of a 3×3 matrix, and obtain analytical expressions.

Following Refs. 3 and 13, we study the frequency dependence of the transmission amplitudes in the limit of small oscillation amplitude ε . We show that there exists a time scale τ , such that the side-band asymmetry (studied by BL) is a function of $\Omega\tau$. This time scale is not the same as the one defined by BL which vanishes in the delta barrier limit. This indicates the possibility of more than one time scale for the tunneling process.

2. MODEL

2.1. Analytical Solution

We consider a time periodic potential (1) where V_0 is the barrier strength, ε ($0 < \varepsilon < 1$) is the modulation strength amplitude, and Ω is the barrier frequency.

We first note that since the problem is periodic the general solution of the wave equation is a superposition of eigenstates of the Floquet operator, i.e., the operator which shifts the solution in time by one period. Thus we can solve for each such eigenstate separately. Since the frequency of the incoming part of the asymptotic behavior of the solution is determined by the incident energy, this energy fixes the corresponding eigenvalue to be $e^{-iE_iT/\hbar}$, where E_i stands for the incident energy. The outgoing parts of the asymptotic solution correspond to the transmitted and reflected particles, and their frequencies must match the same eigenvalue, i.e., $e^{-iE_iT/\hbar} =$ $e^{-iE_iT/\hbar}$, where E_f is the final energy, after transmission or reflection. We thus conclude that the frequency of all the asymptotic outgoing waves should differ from the initial frequency by an integer multiple of Ω , i.e., the energy change is an integer number of energy quanta $\hbar\Omega$.

The corresponding Schrödinger equation is

$$i\hbar\frac{\partial}{\partial t}\psi = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right)\psi \tag{2}$$

On both sides of the barrier the solution of Eq. (2) is just a free particle solution. We thus separate the solution, and write it on both sides as a superposition of free particle functions, satisfying the scattering boundary conditions, and having appropriate frequencies:

$$\psi(x,t) = \begin{cases} \psi_{l}(x,t) = e^{(ik_{0}x - i\omega_{0}t)} + \sum_{n} r_{n}e^{(-ik_{n}x - i\omega_{n}t)}, & x < 0\\ \psi_{r}(x,t) = \sum_{n} t_{n}e^{(ik_{n}x - i\omega_{n}t)}, & x > 0 \end{cases}$$
(3)

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where r_n and t_n are the reflection and transmission coefficients, $\omega_n = (E + nh\Omega)/\hbar$, $k_n = \sqrt{2m\omega_n/\hbar}$, and the summations are over every integer *n*. For negative ω_n , k_n become imaginary, $k_n = i\kappa_n$. The corresponding wave functions cannot be extended to the whole space, but still can contribute to the wave function on one side. One picks the decaying solution to ensure integrability.

Continuity of the wave function requires $\psi_i(0, t) = \psi_i(0, t)$, implying the following relations:

$$r_n = t_n, \qquad n \neq 0$$

$$1 + r_0 = t_0, \qquad n = 0$$
(4)

Integrating Eq. (2) over the barrier region one obtains a tridiagonal matrix equation:

$$(2ik_n/B - 1)r_n - \frac{\varepsilon}{2}(r_{n+1} + r_{n-1}) = \delta_{0,n} + \frac{\varepsilon}{2}(\delta_{0,n+1} + \delta_{0,n-1})$$
(5)

where $B = 2mV_0/\hbar^2$.

In order to solve Eq. (5) we need to invert an infinite matrix. Practically, it is enough to truncate the matrix after about a dozen rows around the center (n=0), since the far r_n 's approach zero quickly (we denote this solution by FS, for full solution). Moreover, it is easy to show that for $|n| \ge 1$ the matrix elements are approximately constant. In this case we can treat our matrix as a Toeplitz matrix,⁽¹⁷⁾ and assume that the solution decays exponentially. The solution is then obtained by inversion of a 3×3 matrix (we call this solution TS for Toeplitz solution).

Let us now focus on the TS. The method of reduction of an infinite approximate Toeplitz matrix into a small finite one has been described elsewhere.⁽¹⁸⁾ We thus only briefly sketch the solution. We have to substitute the exponential correction to the 3×3 matrix; the new matrix equation is

$$\begin{pmatrix} -\frac{\varepsilon}{2}e^{-\theta_{-}} + \frac{2i}{B}k_{-1} - 1 & -\frac{\varepsilon}{2} & 0\\ -\frac{\varepsilon}{2} & \frac{2i}{B}k_{0} - 1 & -\frac{\varepsilon}{2}\\ 0 & -\frac{\varepsilon}{2} & -\frac{\varepsilon}{2}e^{-\theta_{+}} + \frac{2i}{B}k_{1} - 1 \end{pmatrix} \begin{pmatrix} r_{-1}\\ r_{0}\\ r_{1} \end{pmatrix} = \begin{pmatrix} \frac{\varepsilon}{2}\\ 1\\ \frac{\varepsilon}{2} \end{pmatrix}$$
(6)



Fig. 2. Correspondence between FS (full solution) and TS (Toeplitz solution). h=2m=1, $\Omega=\varepsilon=1$, $V_0=10$. (a) $E=2.5>2\Omega$; (b) $\Omega < E=1.5<2\Omega$; (c) $E=0.5<\Omega$; (d) same as (a), but for $\varepsilon=0.5$.



Fig. 2. (Continued)

where θ_{-} and θ_{+} are complex exponents characterizing the (exponential) decay of the t_n 's on both sides of the central energy band, n = 0 ($\Re(\theta_{-}), \Re(\theta_{+}) > 0$). These exponents can be found by assuming that $r_n = r_{-1} \exp((n+1) \theta_{-})$ for $n \leq -1$ and $r_n = r_1 \exp(-(n-1) \theta_{+})$ for $n \geq 1$, and substituting into Eq. (5). We discuss three regimes: (a) $E > 2\hbar\Omega(k_{-1} \text{ and } k_{-2} \text{ are positive})$, (b) $\hbar\Omega < E < 2\hbar\Omega(k_{-1} \text{ positive and } k_{-2} \text{ imaginary})$, and (c) $E < \hbar\Omega(k_{-1} \text{ and } k_{-2} \text{ are imaginary})$. In the first regime the solution is

$$\cos(\mathfrak{J}(\theta_{\pm})) = \frac{\sqrt{2}}{2\varepsilon} \left(1 + \varepsilon^{2} + \frac{4}{B^{2}} k_{\pm 2}^{2} - \sqrt{(1 - \varepsilon^{2})^{2} + \frac{16}{B^{4}} k_{\pm 2}^{4} + \frac{8}{B^{2}} (1 + \varepsilon^{2}) k_{\pm 2}^{2}} \right)^{1/2}$$
$$\cosh(\mathfrak{R}(\theta_{\pm})) = -\frac{1}{\varepsilon} \cos(\mathfrak{J}(\theta_{\pm}))^{-1}$$
(7)

while similar solutions can obtained for cases (b) and (c).

It is clear from Eq. (7) that as ε becomes smaller, the correspondence between FS and TS improves. Since we are interested in the limit $\varepsilon \to 0$, we regard the TS as an exact one. Figure 2 compares the FS and TS in all three cases mentioned before (a-c) when $\varepsilon = 1$, which is the worst case. There is a good agreement for the three central coefficients even in the extreme case of $E \ll (2m/\hbar^2) V_0^2$. Significant relative deviations are obtained only for the levels whose population is exponentially small. Much better correspondence is achieved for smaller ε ; see Fig. 2d. Since in what follows we use only these three coefficients, this figure confirms the accuracy of the Toeplitz method for the following derivation.

2.2. Numerical Results

We verify the above derivation by solving numerically the dynamical time-dependent Schrödinger equation and comparing the results to the FS. In order to simplify the numerical calculation, the delta function barrier is placed in the center of an infinite well. The algorithm we use is as follows. First, we find the eigenfunctions and eigenvalues of the static problem, for each time. Once these are given, the numerical calculation becomes much simpler using adiabatic perturbation theory, leading to a set of first-order differential equations. Due to symmetry, half of the matrix elements vanish. In the case of the delta function the odd eigenfunctions are time independent, and thus the effective number of equations is reduced.² The numerical

² The number of levels taken in the computation should include at least the first few energy bands $\langle E \rangle \pm nh\Omega$.



Fig. 3. Tunneling probability as a function of Ω . Comparison of FS and dynamical computation. The units taken are such that $\hbar = 2m = 1$, $\langle E \rangle = 5$, $V_0 = 5$, $\varepsilon = 0.9$. The inset zooms on the maximum region.

solution is performed using the adaptive time step fifth-order Cash–Karp Runge–Kutta method.⁽¹⁹⁾ The initial wave function is a Gaussian wave packet located in the center of the left side of the barrier, moving toward the oscillating barrier. The wave packet collides with the barrier and splits to reflecting and transmitted parts. We measure the probability to be on the right side of the barrier after a collision.

The same probability is calculated using FS in the following way. We average the transmitted probability current given by FS over the energy, using the weights obtained from the energy components of the initial wave packet taken above. The results of the analytic and numeric results are presented in Fig. 3. The agreement between the two calculations is very good, confirming our derivation.

3. TUNNELING TIME SCALES

In order to investigate the tunneling time problem, one follows the strategy explained above, inspired by BL, and studies the frequency dependence of the transmission intensities in the limit of small ε . In particular, one looks at the relative sideband asymmetry

$$F(\Omega) = \frac{I_1 - I_{-1}}{I_1 + I_{-1}} \tag{8}$$

where $I_n = |t_n|^2$. BL show that for an opaque rectangular barrier, in the high-frequency

$$F(\Omega) = \tanh\left(\frac{m\kappa\Omega}{\hbar d}\right) \equiv \tanh(\Omega\tau_{BL}) \tag{9}$$

where τ_{BL} is defined as the tunneling time. The frequency $\Omega = \tau_{BL}^{-1}$ is the transition frequency below which the behavior is determined by the low-frequency limit.

In the low-frequency limit, BL obtained the relation

$$I_{+} = (\varepsilon V \tau / 2\hbar^2)^2 \tag{10}$$

for an opaque finite barrier, whose height is V. Using this equation as a *definition* of τ , they got the following result for a general barrier:

$$\tau = \left(\frac{m}{\hbar\kappa^2}\right) \left[\frac{(\kappa^2 - k^2)^2 \kappa^2 d^2 + k_0^4 (1 + \kappa^2 d^2) \sinh^2 \kappa d}{+ k_0^2 \kappa d (\kappa^2 - k^2) \sinh 2\kappa d}\right]^{-1/2}$$
(11)

where $\kappa = (2m/\hbar^2)^{1/2} \sqrt{V-E}$, $k_0 = (2mV/\hbar^2)^{1/2}$, $k = (2mE/\hbar^2)^{1/2}$, and *d* is the barrier width. In the delta barrier limit this expression vanishes. The same result is obtained for the general rectangular barrier using the Larmor clock approach.⁽¹¹⁾

In what follows we use the first approach of BL, namely, looking at the asymmetry, and show that for a delta barrier in the deep tunneling regime $E \ll (2m/\hbar^2) V_0^2$, the frequency behavior depends on a new time scale. Using the above-described Toeplitz method, we obtained for the asymmetry function $F(\Omega) = -\Omega \tau_{\delta}$, where

$$\tau_{\delta} = \frac{2\hbar^3}{mV_0^2} \tag{12}$$

This holds only in the regimes (a–b), i.e., when $E > \hbar \Omega$. In the other regime the behavior is also a function of $\Omega \tau_{\delta}$, $f(\Omega) = \sqrt{\Omega \tau_{\delta} - T_0}$, where T_0 is the tunneling probability in the absence of oscillations. Similar results for the model (1) were obtained by Støvneng and Hauge without using the Toeplitz approach.⁽²⁰⁾

One thus sees that following the approach taken by BL, one finds a new and different time scale than the one obtained via the Larmor clock, which was also given in BL's original work using the low-frequency limit. The interpretation of this result is not yet clear. We suggest that there are

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more than one time scale in the tunneling through a general barrier. BL claimed that since, for the opaque barrier, in the high-frequency regime one gets a clear definition of $\tau = \tau_{BL}$ [Eq. (9)] this τ is *the tunneling time* for the opaque barrier. Therefore, looking at the low-frequency regime and knowing the tunneling time, one can extract a connection between the low-frequency behavior and the tunneling time

$$\tau = \frac{2\hbar^2}{\varepsilon V} \sqrt{I_{\pm}} \tag{13}$$

This relation was then used⁽¹³⁾ to define the tunneling time in the general case. Now, if there is more that one time scale in the process, there is no reason to take the time scale which dominates the high-frequency regime and connect it to the low-frequency behavior which may be dominated by a different time scale. Looking at a delta barrier, in which the first time scale τ_{BL} vanishes and only the second time scale plays a role, one indeed sees that both the high- and low-frequency regimes are dominated by the same (second) time scale τ_{δ} .

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