Tunneling times for one-dimensional systems

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(Received 10 June 1994)

We derive a general expression for the tunneling time in layered systems based on the Larmor-clock approach. We show that our results are equivalent to those obtained by the Feynman path-integral technique. We establish a relation between functional derivatives of the barrier potential and partial derivatives with respect to the incident energy. In application, we computed the tunneling time and the reflection time for a rectangular barrier, for a double rectangular barrier and for a Gaussian potential.

I. INTRODUCTION

The question of the time required by a particle to tunnel through a barrier is a long-standing problem, which has raised great interest recently. It is a difficult theoretical problem, which has been approached from many different points of views, as shown in the recent review on the subject by Landauer and Martin.[1] The most direct method to calculate the tunneling time would be to follow the behavior of a wave packet incident on the barrier, but this type of approach is beset with difficulties, mainly associated with the dispersive character of the propagation and with the difficult experimental determination of the delays due to the barrier.[2,3] Physically more significant is the time during which a transmitted particle interacts with the barrier, as measured by some physical clock which can detect the particle's presence within the barrier. One of the principal approaches to this problem is to utilize the Larmor precession frequency of the spin, produced by a weak magnetic field acting within the barrier region. The amount of precession clocks the characteristic tunneling time τ_T, the so-called Büttiker-Landauer time.[4,5] The treatment to obtain τ_T is equally valid for energies higher than the maximum barrier potential and even for negative potentials. In these cases the term traversal time would be more appropriate, but nevertheless we will use uniformly the term tunneling time.

In the next section we derive an expression for the tunneling time in layered systems and show that it is equivalent to those of Sokolovski and Baskin,[6] obtained with the Feynman path-integral technique, and to those of Leavens and Aers,[7] using the auxiliary barrier potential. We establish a relation between functional derivatives of the barrier potential and partial derivatives with respect to the incident energy. We finally apply our results to a rectangular barrier, a double rectangular barrier, and a Gaussian potential.

II. TUNNELING TIME FOR LAYERED SYSTEMS

Gasparian and Pollak,[8] using the Larmor-clock approach, found that the two components of the Büttiker-

Landauer tunneling time for an arbitrary barrier are connected with the integrated density of states and the Landauer resistance and are given by

$$\tau_z = \mathrm{Re} \int_0^L G(x,x)\,dx,$$
$$\tau_y = \mathrm{Im} \int_0^L G(x,x)\,dx, \qquad (1)$$

where $G(x,x)$ is the retarded Green function (GF) of the system. In order to calculate these two time components, we introduce the following general model. Let us consider that our system can be divided into $(N-1)$ layers, labeled $n = 1, ..., N-1$, which are placed between two semi-infinite media. The positions of the boundaries of the nth layer are given by x_n and x_{n+1}. We allow a possible discontinuity in the potential $V_n(x)$ at each boundary between two layers. Let us assume that we know the GF of each layer if the corresponding media were infinite, $G_n^{(0)}(x,x')$, where the index n refers to the layer. The upper index will indicate the number of boundaries considered in the calculation of a given GF. We want to calculate the final GF which incorporates the effects of multiple reflections between layers. To this end we use an exact, nonperturbative, mathematical method, based on the surface Green function method, proposed by García-Moliner and Rubio[9] and by Velicky and Bartoŝ[10] to study the energy spectra of electrons in systems containing interfaces between different crystals. In this method the GF is evaluated first for the case of a single boundary between two media. Then, the case of two boundaries is solved using the GF for one boundary. The problem is solved iteratively for $n + 1$ boundaries, considering that the solution for n boundaries is known.

The GF for the complete system at coinciding coordinates in the nth layer is given by[11]

$$G_n^{(N)}(x,x) = G_n^{(0)}(x,x)\left[1 + R_{n,n-1}^{(n)} R_{n,n+1}^{(-n+N)}\lambda_{n,n+1}\right.$$
$$- R_{n,n-1}^{(n)} e^{2i[\theta_n(x)-\theta_n(x_n)]}$$
$$\left. - R_{n,n+1}^{(-n+N)} e^{2i[\theta_n(x_{n+1})-\theta_n(x)]}\right] D_N^{-1}, \qquad (2)$$

where D_N is a characteristic determinant, $R^{(n)}_{n,n-1}$ is the amplitude of electron reflection from the left block (when an electron enters this block from the right), $R^{(-n+N)}_{n,n+1}$ is the amplitude of electron reflection from the right block (when an electron enters this block from the left), and $\theta_n(x,E)$ is a phase factor. In the Appendix we give the general expressions for all these quantities, and their particular values for piecewise-constant potentials, δ functions, and tight-binding models.

To evaluate τ_y and τ_z we have to integrate Eq. (2) in each layer and sum the contributions of all layers. We can do this for a piecewise-constant potential, as was first done by Aronov et al.[11] The result is

$$\int_0^L G(x,x)\,dx = \sum_{n=1}^{N-1} \frac{\partial \ln t_N}{\partial V_n}. \tag{3}$$

Sokolovski and Baskin[6] applied the Feynman path-integral approach to calculate the tunneling time, and they arrive at the following complex time:

$$\tau_T^{SB} = \int_0^L \frac{\delta \ln t_N}{\delta V(x)}\,dx, \tag{4}$$

where $\delta/\delta V(x)$ is a functional derivative. The modulus of this expression is the time that Büttiker[5] obtained for the tunneling time associated with a Larmor clock in a square potential. Leavens and Aers[12] extended Büttiker's results to a general barrier, and show the equivalence of their results with the results of Sokolovski and Baskin, approximating the functional derivative with respect to the potential by the derivative with respect to the average height of the potential, and keeping the spatial variation of the potential fixed. We can see immediately that Eq. (3) is identical to the modulus of the complex time of Sokolovski and Baskin, Eq. (4), under the following conditions: $N \to \infty$ while keeping L fixed, and replacing the sum by an integral. Equations (3) and (4) are not adequate for practical calculations. Leavens and Aers[12] avoid the problem by approximating the functional derivative with respect to the potential by a partial derivative with respect to the average potential. We can rewrite Eq. (3) exactly in terms of partial derivatives with respect to energy (or, equivalently, incident wave vector $k = \sqrt{E}$). We get

$$\tau_z = \frac{1}{2k}\mathrm{Re}\left\{ \frac{\partial \ln t_N}{\partial k} + \frac{1}{2k}(R^{(N)}_{0,1} + R^{(N)}_{N,N-1}) \right\},$$

$$\tau_y = \frac{1}{2k}\mathrm{Im}\left\{ \frac{\partial \ln t_N}{\partial k} + \frac{1}{2k}(R^{(N)}_{0,1} + R^{(N)}_{N,N-1}) \right\}. \tag{5}$$

This is a general expression, independent of the layer model considered. The complete expressions for t_N, $R^{(N)}_{0,1}$, and $R^{(N)}_{N,N-1}$, obtained with the layer model, are given in the Appendix. The first term on the right-hand side (RHS) of Eqs. (5), proportional to $\partial \ln t_N/\partial k$, mainly contains information about the region of the barrier. Most of the information about the boundary is provided by the reflection amplitudes $R^{(N)}_{0,1}$ and $R^{(N)}_{N,N-1}$, and becomes important for low energies and/or short systems.

The difference between derivatives with respect to the incident energy and with respect to the barrier potential was already considered by Leavens and Aers,[12] by Büttiker,[13] and by Martin and Landauer[14] for a square potential. Leavens and Aers[12] and Büttiker[13] showed that the discrepancy for these two concepts [expressed by our second term on the RHS of Eqs. (5)] can be very large at small energies. We further discuss this question in Sec. IV A.

Martin and Landauer[14] obtained the tunneling time for a modulated incident amplitude in terms of derivatives with respect to incident energy and they pointed out that there is no contradiction with the results obtained by other clock approaches since they correspond to different times.

Gasparian and Pollak[8] obtained for τ_z and τ_y only the first terms on the RHS of the previous equations. Their result is correct in the limit of a very long barrier and not very low energies and in the resonant case, when the influence of the boundaries is negligible.

III. NUMERICAL METHOD

We have developed a program to obtain numerically the tunneling and reflection times as a function of the incident wave vector for any general piecewise-constant potential barrier, for any set of δ functions, and for tight-binding systems. The evaluation of the integrals of the GF can be done with the help of the characteristic determinant.[11] This determinant is made up of the transmission and reflection coefficients of the layers and can be transformed into the determinant of a tridiagonal matrix; so its computation can be done very efficiently.

In the Appendix we give the recursive expression of the characteristic determinant D_N. Once we obtain D_N, it is easy to calculate the transmission amplitude t_N and the reflection amplitudes $R^{(N)}_{0,1}$ and $R^{(N)}_{N,N-1}$, which are the quantities directly entering the computation.

Each time the energy of the particle crosses a potential plateau the numerical calculation becomes very sensitive to the values of the energy considered. We evaluate separately τ_T and τ_R for values of the energy smaller than the plateau and for values bigger than the plateau, and check that there is no discontinuity.

IV. APPLICATIONS

A. Rectangular barrier

The rectangular barrier, which corresponds to our piecewise-constant potential with $N = 2$, was solved analytically by Büttiker[5] considering variations with respect to the potential height. We can obtain the same results from Eq. (5). For this we have to solve the recurrence relation for D_n^0, Eq. (A3), for the case $N = 2$ and calculate $t_2 = 1/D_2$ and $R^{(2)}_{01}$. We find

$$t_2 = 2\Gamma k\kappa \left[2k\kappa \cosh \kappa d + i(\kappa^2 - k^2)\sinh \kappa d \right] \tag{6}$$

and for the amplitude of reflection

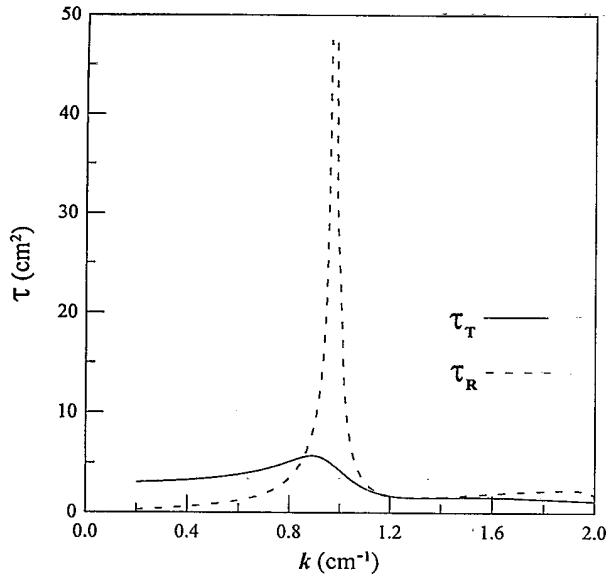FIG. 1. Tunneling time τ_T and reflection time τ_R, as a function of incident wave vector, for a double rectangular barrier. The values of the parameters are $V_0 = 1$, $d_1 = 1$, and $d_2 = 1.5$.

FIG. 2. Tunneling time τ_T and reflection time τ_R, as a function of incident wave vector, for a Gaussian barrier of height equal to 1 and width equal to 6.

$$R_{01}^{(2)} = -V_0\Gamma[(\kappa^2 - k^2)\sinh\kappa d + 2ik\kappa\cosh\kappa d]\sinh\kappa d. \tag{7}$$

Leavens and Aers[12] obtained $\tau_y^{(E)}$ and $\tau_z^{(E)}$ in a square potential by considering variations of the incident energy, as suggested by Büttiker and Landauer.[15] In our notation, the result is

$$\tau_y^{(E)} = \tau_y^{\mathrm{BL}} - \frac{1}{2k^2}\mathrm{Im}R_{0,1}^{(2)},$$

$$-\tau_z^{(E)} = \tau_z^{\mathrm{BL}} - \frac{1}{2k^2}\mathrm{Re}R_{0,1}^{(2)}. \tag{8}$$

As this difference in the tunneling time is proportional to the amplitude of reflection, we conclude that it arises from boundary effects.

B. Double rectangular barrier

We now apply our results to a double rectangular barrier, $N = 4$. Let us call the height of the barrier potentials V_0 and their width d_1. The distance between the barriers is d_2.

In Fig. 1 we represent τ_T and τ_R as a function of k for a double rectangular barrier. We choose our parameters so that there is only one quasibound state per well. The parameters are $V_0 = 1$, $d_1 = 1$, $d_2 = 1.5$. The resonance corresponds to $k = 0.977$. We can see in Fig. 1 that in resonance the reflection time exhibits a maximum.

C. Gaussian barrier

We have applied our method to a Gaussian barrier, which is approximated by a piecewise-constant potential with a different number of steps. In Fig. 2 we represent the tunneling time (short-dashed line) and the reflection
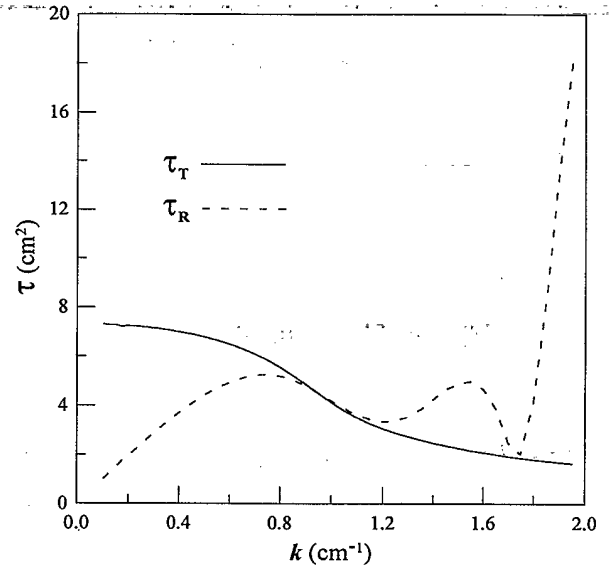
time τ_R (long-dashed line), as a function of incident wave vector. The height of the barrier is equal to 1 and its spread is equal to 6. The figure corresponds to $N = 10$, but the results are basically indistinguishable from those corresponding to higher values of N.

V. CONCLUSIONS

To conclude, we would like to stress that the GF method, which is not a perturbation approach, is very appropriate for practical calculations of tunneling times. Although our results are based on the Larmor-clock approach, there are indications that they can be applicable to a wide range of clocks.

ACKNOWLEDGMENTS

APPENDIX: CHARACTERISTIC DETERMINANT

The amplitude of transmission through a multilayered structure is inversely proportional to the characteristic determinant, $t_N = D_N^{-1}$, which can be expressed as the product

$$D_N = D_N^0\left\{\prod_{n=1}^{N}\lambda_{n-1,n}(1 - r_{n,n-1})(1 - r_{n-1,n})\right\}^{-1/2}, \tag{A1}$$

where the factor $\lambda_{0,1}$ is defined as equal to 1. The quantity $r_{n-1,n}$ ($r_{n,n-1}$) is the amplitude of the reflection of the electron propagating from the region $n-1$ into n (n into $n-1$). The quantity $\lambda_{n-1,n} = \lambda_{n,n-1}$ is defined by

$$\lambda_{n-1,n} = \int_{x_n}^{x_{n+1}} \frac{i\,dx}{2G_n^{(0)}(x,x)}. \qquad (A2)$$

D_N^0 is the determinant of a tridiagonal matrix and satisfies the following recurrence relationship:

$$D_n^0 = A_n D_{n-1}^0 - B_n D_{n-2}^0, \qquad (A3)$$

where $A_1 = D_0^0 = 1$, $D_1^0 = 0$, and we have for $n > 1$

$$A_n = 1 + \lambda_{n-1,n} \frac{r_{n-1,n}}{r_{n-2,n-1}} (1 - r_{n-2,n-1} - r_{n-1,n-2}) \qquad (A4)$$

and

$$B_n = \lambda_{n-1,n} \frac{r_{n-1,n}}{r_{n-2,n-1}} (1 - r_{n-2,n-1})(1 - r_{n-1,n-2}). \qquad (A5)$$

The reflection amplitude $R_{N,N-1}^{(N)}$ may also be written in the form

$$R_{N,N-1}^{(N)} = \frac{\tilde{D}_{N+1}^0}{D_N^0}, \qquad (A6)$$

where $\tilde{D}_{N+1}^0$ is given by

$$\tilde{D}_{N+1}^0 = \frac{(1 - r_{N,N-1} - r_{N-1,N})}{r_{N-1,N}} D_N^0 - \frac{(1 - r_{N,N-1})(1 - r_{N-1,N})}{r_{N-1,N}} D_{N-1}^0. \qquad (A7)$$

$R_{0,1}^{(N)}$ can be written in a similar way. In the case of a symmetric barrier, we have $R_{0,1}^{(N)} = R_{N,N-1}^{(N)}$.

The values of $r_{n,n-1}$ are model dependent. For a piecewise-constant potential we have

$$r_{n,n-1} = -\frac{G_n^{(0)}(x_n,x_n) - G_{n-1}^{(0)}(x_n,x_n)}{G_n^{(0)}(x_n,x_n) + G_{n-1}^{(0)}(x_n,x_n)}, \qquad (A8)$$

and $r_{n-1,n} = -r_{n,n-1}$. For a tight-binding model and for a set of δ functions, we obtain

$$r_{n,n-1} = \frac{-V_n G_n^{(0)}}{1 + V_n G_n^{(0)}} \qquad (A9)$$

and $r_{n-1,n} = r_{n,n-1}$, where V_n is the nth diagonal energy in the tight-binding case, and the strength of the nth δ function in the other case. $G_n^{(0)}(x,x)$ is the unperturbed GF, for each case.

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