Büttiker-Landauer characteristic barrier-interaction times for one-dimensional random layered systems

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This paper derives expressions for tunneling time through random one-dimensional barriers consisting of an arbitrary sequence of δ-function scattering potentials with an arbitrarily varying spacing, and an arbitrarily varying strength from potential to potential. The tunneling times are derived in the spirit of Baz's idea to utilize a Larmor precession clock. A physical connection is made between the y and z components of the Büttiker-Landauer tunneling times, the density of states, and the Landauer resistance, respectively. A simple extension of the usual time-independent treatment provides further insight into the significance of the two components.

I. INTRODUCTION

Recently there has been considerable interest[1] in the subject of tunneling through one-dimensional potential barriers. Different approaches and definitions exist for the tunneling times. There is a good recent review on the subject by Hauge and Støveng.[2] The most extensively studied is the so-called Büttiker-Landauer time,[3] based on an idea by Baz[4] to utilize the Larmor procession frequency of the spin (in the weak magnetic fields) as a clock for such times. In this method, the spin is thought to be polarized initially along the direction of travel of the electron (x direction). The rotation of the spin, as it traverses the barrier, is then studied by determining the time evolution of its z component along the magnetic field transverse to x, and along its y direction. Two times, τ_y and τ_z, are then determined as the inverse expectation values of the y and z components, respectively, of the Larmor frequency.

In this paper we find a connection between τ_y and τ_z, and between some other simple properties of the barrier. Specifically, it is shown that τ_y is proportional to the density of states, and thus simply related to a group velocity, and τ_z is a simple function of the Landauer resistance of the barrier.

The paper also calculates τ_y and τ_z for types of barriers for which they have not yet been calculated. To our knowledge, all previous work on the subject dealt with the relatively simple case of single- or double-square potential barriers. Here we treat a type of barrier $V(x)$ which is an arbitrarily long sequence of δ-function potential, with the possibility of disorder in their spacing, as well as in their strengths,

$$V(x)=\sum_{j=1}^{N} V_j\delta(x-x_j),\quad x_j<x_{j+1}$$

where V_l is the strength of the lth δ potential and x_n the coordinate of the nth δ potential. The calculations are based on a method of evaluation by Gasparian, Al'tshuler, Aronov, and Kasamanian,[5] and by Gasparian[6] for the evaluation of the transmission coefficient T from the determinant D_N, defined by

$$D_N=\det[\delta_{jl}+(iV_l/2k)\exp(ik|x_j-x_i|)]\ ,\qquad j,l=1,2,\ldots,N\ ,$$

where k is the value of the wave vector of the incident particle.

II. DERIVATION OF THE PRINCIPAL EXPRESSIONS

In this section we derive a relationship between the tunneling time of an electron through a one-dimensional random system with determinant D_N, using the Baz[4] method. We consider a one-dimensional random potential $V(x)$ in a finite segment $0<x<L$. Let us propose that a weak magnetic field $\mathbf{B}=B\theta(x)\theta(L-x)\hat{z}$, pointing in the z direction, and confined to the (arbitrary) barrier. An electron is incident from the left on the barrier. It carries spin $s=\frac{1}{2}$, polarized at $x=0$ in the x direction, i.e., $\langle s_x\rangle=\frac{1}{2}$, $\langle s_y\rangle=0$, $\langle s_z\rangle=0$.

The spinor $\Psi(L)$, in the lowest order in B, will be presented in the form

$$\Psi(L)=\begin{bmatrix}1\\1\end{bmatrix}\Psi_0(L)+\frac{B}{2}\begin{bmatrix}1\\-1\end{bmatrix}\int_0^L dx\ \Psi_0(x)G(L,x)\ . \quad (1)$$

Here $\Psi_0(x)$ is the solution of the Schrödinger equation when $B=0$:

$$\Psi_0(x)=\exp(ikx)-\int_0^L G(x,x')V(x')\exp(ikx')dx'\ .$$
$$=ikG(0,x),\quad k=(E+i\epsilon)^{1/2}$$

($\hbar=1$, and $m_0=\frac{1}{2}$ is the electron mass). The Green function (GF) $G(x,x')$ should satisfy the Dyson equation

$$G(x,x')+\int_0^L G_0(x,x'')V(x'')G(x'',x')dx''=G_0(x,x')\ ,$$

where $G_0(x,x')=\exp(ik|x-x'|/2ik)$ is the free-electron GF.

As the electron enters the random barrier, it starts the Larmor precession with frequency $\omega_L=g\mu B/\hbar$ (g is the gyromagnetic ratio and μ the absolute value of the magnetic moment). When the electron leaves the disordered

barrier the precession stops, and we find [using Eq. (1)] for the orientation of the spins of the transmitted electron

$$\langle s_z\rangle = 4B|\Psi_0(L)|^2 \mathrm{Re}\int_0^L G(x,x)dx \ ,$$
$$\langle s_y\rangle = 4B|\Psi_0(L)|^2 \mathrm{Im}\int_0^L G(x,x)dx \ , \tag{2}$$
$$\langle s_x\rangle = 2|\Psi_0(L)|^2\left[1-B^2\left|\int_0^L G(x,x)dx\right|^2\right] .$$

The derivation of Eqs. (2) made use of the relation[5] connecting $G(x,x')$ with the one-particle GF at the coinciding coordinates $x=x'$:

$$G(x,x') = [G(x,x)G(x',x')]^{1/2} \times \exp\left[-\int_{\min(x,x')}^{\max(x,x')} dx_1/2G(x_1,x_1)\right] ,$$

Note that the integral of the type

$$\int_0^L G(x,x)dx$$

in Eqs. (2) can be evaluated quite generally[6] by

$$\int_0^L G(x,x)dx = \partial[\ln D_L(E)]/\partial E \ . \tag{3}$$

The function $D_L(E)$ in fact describes the energy spectrum of the random system by $D_L(E_n)=0$, and is connected with the coefficient of transmission of an electron by the relationship $T_L|D_L(E)|^{-2}$. It is possible to obtain explicit expressions for the function $D_L(E)$ in each specific case (the case of a sequence of δ-function potentials with arbitrary amplitudes V_l at arbitrary points x_l is considered in Ref. 5; the case of a randomly layered system is considered in Ref. 6).

Using Eq. (2) and $\langle s_x\rangle^2+\langle s_y\rangle^2+\langle s_z\rangle^2=\frac{1}{4}$ we obtain from Eq. (1), for $\langle\tau_x\rangle$, $\langle\tau_y\rangle$, and $\langle\tau_z\rangle$, in the limit of an infinitesimal field B,

$$\tau_z = \mathrm{Re}(\partial \ln D_L/\partial E) \ ,$$
$$\tau_y = -\mathrm{Im}(\partial \ln D_L/\partial E) \ , \tag{4}$$
$$\tau_x = \{[\mathrm{Re}(\partial \ln D_L/\partial E)]^2+[\mathrm{Im}(\partial \ln D_L/\partial E)]^2\}^{1/2} .$$

Making use of a relation[6] which connects the determinant D_L and the one-dimensional average electronic density of states $\nu_L(E)$,

$$-\mathrm{Im}(\partial \ln D_L/\partial E) = \pi L \nu_L(E) \ ,$$

and the relation between D_L and Landauer's resistance[5] $\rho_L(E)$,

$$\rho_L(E) = |D_L(E)|^2 - 1 \ ,$$

we can obtain from Eq. (4)

$$\tau_z = 1/2\{\partial \ln[\rho_L(E)+1]/\partial E\} \ ,$$
$$\tau_y = \pi L \nu_L(E) \ . \tag{5}$$

Büttiker[3] introduced the expression of τ_y and τ_z in terms of a barrier height derivative of

$$\tau_x = (\tau_y^2+\tau_z^2)^{1/2} \ ,$$

the complex transmission coefficient of an electron through a rectangular barrier. The representation of τ_z and τ_y as the real and imaginary parts of the energy derivative of the complex electron transmission coefficient, through an arbitrary barrier, were introduced by Leavens and Aers.[7] But, to our knowledge, this is the first time that τ_y and τ_z are expressed, respectively, in terms of the density of states, and of the Landauer resistance of a one-dimensional random system. Equations (5) are the main result of our paper.

As Thouless has shown,[8] a dispersion relation exists between the localization length and the density of states. This relation can be expressed[5] in the form of a linear dispersion relation between $\ln|D_N|$ and the imaginary part $\mathrm{Im}\ln D_N$. The self-averaging property of τ_y and of τ_z is therefore an immediate consequence of self-averaging of the localization length and of the density of states.[5]

Let us calculate τ_y and τ_z in the general case of N arbitrarily spaced δ potentials V_l in a chain which has a finite length. In this case the elements of the determinant D_N have the form[5]

$$(D_N)_{nl} = \delta_{nl} + (iV_l/2k)\exp(ik|x_l-x_n|) \ . \tag{6}$$

Here $|x_l-x_n|$ is the distance between the lth and the nth δ potential.

The determinant $D_N \equiv \mathrm{Det}|D_{nl}|$ satisfies the following recursion relation:

$$D_N = A_N D_{N-1} - B_N D_{N-2} \ , \tag{7}$$

where D_{N-n} is the determinant of the matrix of Eq. (6), without the $(N-n-1)$th row and column,

$$D_0 = 1, \quad D_{-1} = 0 \ ,$$
$$B_N = \exp(2ik|x_N-x_{N-1}|)(V_N/V_{N-1}) \ ,$$
$$A_1 = 1+(iV_1/2k) \ ,$$
$$A_{N>1} = 1+B_N+[1-\exp(2ik|x_N-x_{N-1}|)(iV_N/2k)] \ .$$

For the Krönig-Penney model (N identical and evenly spaced δ potentials) we obtain from Eq. (7),

$$D_N = \cos N\beta a + i[(V/2k)\cos ka - \sin ka]\sin N\beta a/\sin\beta a \ , \tag{8}$$

where a is the lattice spacing and β plays the role of quasimomentum, and is defined by $\cos\beta a = \cos ka + (V/2k)\sin ka$. The condition $|\cos\beta a|>1$ determines the states in the allowed energy band. In this case (as expected) it follows from Eqs. (5) and (8) that

$$\tau_y \simeq (Na/k)(\partial\beta/\partial k)|_{\mathrm{Im}\beta\to+0} \tag{9}$$

and

$$\tau_z \simeq -k^{-1}(\partial \ln|\sin\beta a|/\partial k) \tag{10}$$

as $Na\to\infty$. It can be seen from Eq. (9) that $ka=n\pi$ at the upper edges of the allowed zones [while at the lower edges $ka=n\pi+2\arctan(V/2k)$]; for $k\le n\pi/a$, τ_y increases as $(n\pi/a-k)^{-1/2}$.

For states in the gap (where $\cos i\beta a \equiv \cosh\beta a > 1$) we

find for τ_y and τ_z at $Na \to \infty$, using Eqs. (5) and (8),

$$\tau_y \simeq (1/V)\cosh\beta a[\cos ka - (2k/V)\sin ka](\partial\beta/\partial k) ,$$

$$\tau_z \simeq [Na(\partial\beta/\partial k) - \partial \ln|\sinh\beta a|/\partial k - k^{-1}]/k .$$

Using Eqs. (5) and (8) we obtain for τ_y and τ_z, for arbitrary N,

$$\tau_y = \left\{2k|D_N|^2\left[1+\left[\frac{V}{2k\sin\beta a}\right]^2\right]^{1/2}\right\}^{-1/2}\left\{Na\left[1+\left[\frac{V}{2k\sin\beta a}\right]^2\left[1-\cot\beta a\frac{\sin 2N\beta a}{2N}\right]\right]\frac{\partial\beta}{\partial k}\right.$$
$$\left. - \left[\frac{V}{2k\sin\beta a}\right]^2\frac{\sin 2N\beta a}{2k}\right\} , \tag{11}$$

$$\tau_z = \frac{|D_N|^2-1}{2|D_n|^2k^2}\left[(Nak\cot N\beta a - ak\cot\beta a)\frac{\partial\beta}{\partial k} - 1\right] , \tag{12}$$

where $|D_N|^2 = 1+(V/2k)^2(\sin^2 N\beta a/\sin^2\beta a)$. The corresponding results for τ_y and τ_z for states in the forbidden gap are obtained replacing β by $i\beta'$ ($\beta' > 1$).

For the tunneling case when $\beta = m\pi/Na$ $[m = 1,2,\ldots,(n-1)]$ the transmission coefficient of an electron, $T_N = [1+(V/2k)^2(\sin^2 N\beta a/\sin^2\beta a)]^{-1}$, has an oscillating dependence on the Fermi level, and $T_N = 1$ $N-1$ times in each allowed band. The time τ_y for such β is

$$\tau_y = \frac{Na}{2}\left\{\frac{1}{k}\left[1+\left[\frac{V}{2k\sin\beta}\right]^2\right]^{1/2}\frac{\partial\beta}{\partial k}\bigg|_{\beta=m\pi/Na}\right\} ,$$

$$\tau_{y_1} < \tau_{y_2} < \cdots < \tau_{y_{N-1}} .$$

It is interesting to note from Eq. (11) that τ_y oscillates with energy about the geometric mean result $(Na/2k)(\partial\beta/\partial k)$:

$$[(\tau_y)_{\sin N\beta a=0}(\tau_y)_{\sin N\beta a=1}]^{1/2} = (Na/2k)(\partial\beta/\partial k) .$$

If δ potentials of random strengths are arranged periodically, $x_n = na$, the recurrence relation Eq. (7) can be solved, because at $V_i \sin ka/ka \gg 1$ the values A_1 and $A_{N>1}$ are equal,

$$A_1 \simeq iV_l/2k ,$$

$$A_{N>1} \simeq (V_n/k)\exp(ika)\sin ka$$

and $D_{N-2} \ll D_N$. As a result, we obtain

$$D_N \simeq \frac{i}{\sin ka}\left[\frac{\sin ka}{k}\right]^N\prod_{j=1}^{N}V_j ,$$

and

$$\tau_y = 0 , \tag{13}$$

and

$$\tau_z \simeq [(N-1)/2k][\partial \ln(\sin ka/ka)/\partial k] - 1/2k^2 . \tag{14}$$

We note that Eqs. (13) and (14) are similar for the model in which both the spacing and the strength of the δ potentials fluctuate. For that case we find

$$\tau_y = 0 ,$$

$$\tau_z \simeq [(N-1)/2k][\partial\langle \ln(\sin k\bar{a}/k\bar{a})\rangle/\partial k] - 1/2k^2 ,$$

where $\bar{a}$ is the average distance between two δ potentials.

III. A PHYSICAL COMMENT

The usual procedure to calculate τ_y and τ_z (when the latter is calculated) is to assume a sharply defined k vector. While there is no particular problem in executing such a calculation by calculating the spin rotation and the Larmor frequency, one may nevertheless feel somewhat uncomfortable about the fact that a sharply defined k vector represents a stationary process—what meaning has a tunneling *time* for a stationary process? Any direct experiment of a transition time will *per force* not correspond to a stationary process. It is not necessarily obvious that experimental measurements of a transit time in such a nonstationary process must agree with the calculation obtained on a stationary process.

To alleviate to some degree such questions, we generalize the procedure to a quasistationary process, where the energy is complex, $E = E_0 + i\Gamma$, so that the time dependence $\exp(iE_0t/\hbar)\exp(-\Gamma t/\hbar)$ exhibits an exponential decay with the decay time $\Gamma/\hbar$. In addition to the (we believe) greater physical appeal of such a procedure, it also results in a physical insight into the Büttiker-Landauer time $\tau_x = (\tau_y^2+\tau_z^2)^{1/2}$. We have

$$\tau_y = L\nu(E) = L\,\mathrm{Im}[\partial(\ln D)/\partial E]$$
$$= L\,\mathrm{Im}[(1/D)(\partial D/\partial E)] ,$$

$$\tau_z = L\,\mathrm{Re}[(1/D)(\partial D/\partial E)] .$$

If now $\Gamma \ll E_0$, we can expand

$$D(E) = D(E_0) + (\partial D/\partial E)(E-E_0) + \cdots ,$$

so

$$\tau_y = L\,\mathrm{Im}[(E-E_0-i\Gamma)^{-1}] = L\Gamma/[(E-E_0)^2+\Gamma^2] ,$$

$$\tau_z = L\,\mathrm{Re}[(E-E_0-i\Gamma)^{-1}]$$
$$= [L(E-E_0)]/[(E-E_0)^2+\Gamma^2] ,$$

$$\tau_x=(\tau_y^2+\tau_z^2)^{1/2}=L/[(E-E_0^2)+\Gamma^2]^{1/2} .$$

We notice that when E is at the center of the resonance, τ_x is just $1/\Gamma$.

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