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Büttiker–Landauer tunneling time through one-dimensional barriers of arbitrary shape

VLADIMIR GASPARIAN†
Departamento de Electronica y Tecnologia de Computadores,
Campus de Fuentenueve, Universidad de Granada, Granada, Spain

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A convenient formalism, based on the surface Green's functions is developed that allows one to obtain a general expression for the Büttiker–Landauer tunneling time through one-dimensional barriers of arbitrary shape. It is shown that transmission, reflection and dwell times can be expressed in terms of the scattering-matrix elements. Although the results are based on the Larmor clock approach, there are indications that they will be applicable to a wide range of clocks. A relation between functional derivatives of the barrier potential and partial derivatives with respect to the incident energy is established. Finally, an analytical expression for escape time of an electron from a finite disordered region is derived and the connection to the *local scattering-matrix elements* is discussed.

Key words: tunneling, reflection and escape times, disordered system.

1. Introduction

The calculation of the time interval during which a particle interacts with the barrier of arbitrary shape has raised great interest recently and has been studied both theoretically and experimentally (see, e.g. [1, 2] and references therein). This is of particular importance in the context of the remarkable developments in the fabrication of mesoscopic devices [3, 4] and the synthesis of promising chemical nanostructures [5], where quantum transport is based on the tunneling process. Over the years the problem of tunneling in one-dimensional (1D) systems has been approached from many different points of view, as shown in the recent review on the subject by Landauer and Martin [2]. One approach is to follow the behavior of a wavepacket incident on the barrier and calculate the delay introduced by the barrier. 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]. Physically more significant is the time during which a transmitted particle interacts with the barrier, as measured by some physical clocks which can detect the particle's presence within the barrier. There is a wide choice for the physical clocks [6–12]: one of them, the time-modulated barrier, was proposed by Büttiker and Landauer, to analyze the behavior of transmitted electrons through a potential barrier, supplemented by a small oscillatory perturbation [7, 13]. Another physical clock mechanism, based on an idea by Baz' [6] to utilize the Larmor precession frequency of the spin, produced by a weak magnetic field acting within the barrier region is the so-called Büttiker–Landauer (BL) time τ^{BL} [7, 8]. In this method, which is the most extensively studied, the spin is thought to be polarized

† Permanent address: Department of Physics, Yerevan State University, 375049, Yerevan, Armenia.

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initially perpendicular to the direction of motion of the electron (y-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 perpendicular to y, and along the y-direction. Two times, τ_y^{BL} and τ_z^{BL}, are determined as the inverse expectation values of the y and z components, respectively, of the Larmor frequency. A physical connection was made between the y and z component of the BL tunneling times, the density of states and the Landauer conductance, respectively [14].

This work will concentrate on the Larmor clock approach and following [14, 15], a general expression will be presented for the tunneling and reflection times in terms of the surface of Green's function (GF) of the whole system, including the 1D arbitrary barrier and the regions outside it. Thus a relation between functional derivatives of the barrier potential and partial derivatives with respect to the incident energy is established and an analytical expression for escape time of an electron from a finite disordered region is derived. Furthermore in Appendixes A and B specific expressions for the tunneling time in layered systems are established and it is shown that they are equivalent to those by Sokolovski and Baskin [10], obtained with the Fenman path-integral technique, to those by Leavens and Aers [16], using the auxiliary barrier potential and to those by Jauho and Jonson [17], obtained in the generalized discussion of the time-modulated barrier (see [7, 13]).

2. Formalism in terms of Green's functions

Let us now derive a general expression for the Büttiker–Landauer traversal time using the surface GF method [14, 15]. The GF method, allowing us to take into account multiple interfaces consistently and exactly without the use of the perturbation theory, was proposed in [18, 19] to study the energy spectra of electrons in systems containing interfaces between different crystals (see Appendixes A and B).

We will consider a 1D system with an arbitrary potential $V(y)$ confined to a finite segment $0 < y < L$. We will call this region 'the barrier' of length L, and we will assume that scattering in it is purely elastic. As in the case of a rectangular barrier, discussed by Büttiker [8], we apply a weak magnetic field $\boldsymbol{B}$ in the z-direction and confined to the barrier:

$$\boldsymbol{B} = B\theta(y)\theta(L-y)\hat{\boldsymbol{z}} \tag{2.1}$$

If we concentrate on the motion of an electron, with kinetic energy $E = k^2$ ($\hbar = 1$ and $m = \frac{1}{2}$ is the electron mass) and with spin $s = \frac{1}{2}$, we have to consider its two wavefunctions Ψ_1 and Ψ_2, corresponding to the two spin projections of $+\frac{1}{2}$ and $-\frac{1}{2}$ along the z-axis. The column wavefunction $\hat{\Psi}(y)$ represents compactly both spin states:

$$\hat{\Psi}(y) = \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix}. \tag{2.2}$$

The electron inside the barrier from the left with an energy E and with its spin polarized along the y-direction, has its wavefunction before the barrier given by:

$$\hat{\Psi}(y) = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \exp(iky) \tag{2.3}$$

where $k = (E + i\eta)^{1/2}$, with $\eta \to 0$.

In the presence of a magnetic field, the Schrödinger equation takes the form:

$$\left(-\frac{d^2}{dy^2} + V(y) - E\right)\hat{\Psi}(y) = -\vec{\mu}\boldsymbol{B}\hat{\Psi}(y) = -\mu B \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\hat{\Psi}(y). \tag{2.4}$$

The term $-\vec{\mu}\boldsymbol{B}$ on the right-hand side describes the interaction. Since by assumption the vector $\boldsymbol{B}$ is directed along the z-axis and the magnetic moment $\vec{\mu}$ is of the form $\vec{\mu} = 2\mu\boldsymbol{s}$, where $\boldsymbol{s}$ is the particle spin vector, we

have:

$$\vec{\mu}\boldsymbol{B} = 2\mu s_z B = \mu\sigma_z B = \mu B \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2.5}$$

where σ_z is a Pauli matrix.

The problem is solved by perturbation theory. In the lowest order in B, the spinor $\Psi(L)$ of the electron on the right end of the barrier is given by:

$$\Psi(L) = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \Psi(L) + \frac{B}{2} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \int_0^L \psi(0) G(L, 0)\, dy. \tag{2.6}$$

Here $\psi(y)$ is the solution of the spatial part of the Schrödinger equation in the absence of the magnetic field. This spatial part of the wavefunction can be written in terms of GF of the system as:

$$\psi(y) = \exp(iky) - \int_0^L G(y, y') V(y') \exp(iky')\, dy', \tag{2.7}$$

where $G(y, y')$ is the retarded GF, whose energy dependence is not written explicitly. It should satisfy the Dyson equation:

$$G(y, y') = G_0(y, y') + \int_0^L G_0(y, y'') V(y'') G(y'', y')\, dy'', \tag{2.8}$$

where $G_0(y, y') = i \exp(ik|y - y'|)/2k$ is the free-electron GF. Some properties of the GF are discussed in Appendix A.

2.1. Tunneling time

Now we are ready to obtain all the relevant properties of the problem in terms of the GF solution of the previous equation. The expectation value of the component of the spin along the direction of the magnetic field of the transmitted electron is, up to second order in B:

$$\langle S_z \rangle_T = \tfrac{1}{2} \langle \Psi(L) | \sigma_z | \Psi(L) \rangle = -4B \,\mathrm{Re} \left[\psi^*(L) \textstyle\int_0^L \psi(y) G(L, y)\, dy \right]. \tag{2.9}$$

We want to express the wavefunction $\psi(y)$ appearing inside the integral in the previous equation in terms of the GF. So, we take into account the following relationship between the wavefunction and the GF of a 1D system:

$$\psi(y) = -2ikG(0, y). \tag{2.10}$$

For 1D systems also, we can further simplify the problem by writing the general expression of the GF, $G(y, y')$, in terms of its own expression at coinciding coordinates $y = y'$ [20]:

$$G(y, y') = [G(y, y) G(y', y')]^{1/2} \exp[i|\theta(y) - \theta(y')|], \tag{2.11}$$

where the phase factor $\theta(y, E)$ is defined as:

$$\theta(y, E) = \int \frac{i\, dy}{2G(y, y)}. \tag{2.12}$$

Substituting (2.11) into (2.9) and making use of the relation (2.10) one finds the spin component along the direction of the magnetic field:

$$\langle S_z \rangle_T = 4B |\psi(L)|^2 \,\mathrm{Re} \int_0^L G(y, y)\, dy. \tag{2.13}$$

A similar procedure for the spin component along the y- and x-directions lead to

$$\langle S_y\rangle_T = -4B|\psi(L)|^2 \operatorname{Im}\int_0^L G(y,y)\,dy \tag{2.14}$$

and

$$\langle S_x\rangle_T = 2|\psi(L)|^2\left(1 - B^2\left|\int_0^L G(y,y)\,dy\right|^2\right). \tag{2.15}$$

The z, y and x components of the BL traversal time are proportional to the corresponding spin components [6, 8], and we finally arrive at:

$$\tau_{z,T}^{\mathrm{BL}} = \operatorname{Re}\int_0^L G(y,y)\,dy, \tag{2.16}$$

$$\tau_{y,T}^{\mathrm{BL}} = \operatorname{Im}\int_0^L G(y,y)\,dy, \tag{2.17}$$

and so

$$\tau_T^{\mathrm{BL}} = \left|\int_0^L G(y,y)\,dy\right|, \tag{2.18}$$

if we make use of the following relationship:

$$\langle S_x\rangle^2 + \langle S_y\rangle^2 + \langle S_z\rangle^2 = \tfrac{1}{4}.$$

The final result, eqn (2.16) or eqn (2.17), only depends on the integral of the GF at coinciding coordinates and can be calculated quite generally in a finite region [20, 15]. It is straightforward to show that the final result can be expressed in terms of partial derivatives with respect to energy (or, equivalently, the incident wavevector $k = \sqrt{E}$) (see Appendix B)

$$\tau_{y,T}^{\mathrm{BL}} = \operatorname{Im}\int_0^L G(y,y)\,dy = \operatorname{Im}\frac{1}{2k}\left\{\frac{\partial \ln t}{\partial k} + \frac{1}{2k}(r + r')\right\} \tag{2.19}$$

$$\tau_{z,T}^{\mathrm{BL}} = \operatorname{Re}\int_0^L G(y,y)\,dy = \operatorname{Re}\frac{1}{2k}\left\{\frac{\partial \ln t}{\partial k} + \frac{1}{2k}(r + r')\right\}. \tag{2.20}$$

These are general expressions, independent of the model considered. r and r' are the reflection amplitudes from the left and from the right, respectively. t is the transmission amplitude, which is independent of incident direction as can be deduced from the time reversal and current conservation requirements [21]. For a spatially symmetric barrier $V(y) = V(-y)$ one has additionally $r = r'$.

The first term on the right-hand side of eqns (2.19) and (2.20) proportional to imaginary and real parts of $\partial \ln t/\partial k$, mainly contains information about the region of the barrier. Most of the information about the boundary is provided by the reflection amplitudes r and r', and is of the order of the wavelength λ over the length of the system L, i.e. $0(\lambda/L)$. Thus, it becomes important for low energies and/or short systems. As is pointed out in [22] a calculation of the density of states (DOS) without taking into account the extra term in eqn (2.19) yields a wrong result without an oscillation term. Such oscillations in DOS and the partial DOS should influence the conduction properties of sufficiently small conductors [23].

Note that the second term in eqns (2.19) and (2.20) can be neglected in the semiclassical (WKB) case, if r (and so r') is negligible (e.g., in the resonant case, when the influence of the boundaries is negligible) and, of course when $\lambda \ll L$. When boundary effects can be neglected, such a situation arises in the general analysis of two interfering incident waves, which yields the characteristic time [24]

$$\tau = \hbar|t_E^{-1}|\left|\frac{dt_E}{dE}\right| = \left\{\left(\frac{d\varphi}{dE}\right)^2 + \left(\frac{d\ln T}{dE}\right)^2\right\}^{1/2},$$

as well as in [25], where Leavens and Aers regarded the shape distortion of the transmitted wave by the infinitely large barrier, following the papers of Büttiker and Landauer [13, 26].

The integral of the GF at coinciding coordinates, and so the components of the traversal time, can be related to the density of states and the conductance. It is well known that the imaginary part of $G(y, y)$ is proportional to the local DOS at the corresponding energy. So, $\tau_{y,T}^{\mathrm{BL}}$ (2.19) can also be written in terms of the average DOS of the electron in the system per unit energy and per unit length $\nu_L(E)$:

$$\tau_{y,T}^{\mathrm{BL}} = \pi L \nu_L(E). \tag{2.21}$$

As for the second component of the BL time $\tau_{z,T}^{\mathrm{BL}}$ it can be connected with the conductance of a 1D structure coupled by two perfect leads. Using the well-known Landauer formula for the conductance [27]

$$G = T$$

measured in natural units ($2e^2/h = 1$), we can rewrite eqn (2.20) in the form

$$\tau_{z,T}^{\mathrm{BL}} = \frac{1}{2k}\left\{\frac{\partial \ln G}{2\partial k} + \frac{\sqrt{1-G}}{k}\sin(\varphi)\cos(\varphi_a)\right\}. \tag{2.22}$$

Here φ is the scattering phase and φ_a is an extra phase accumulated, with respect to transmitted particles, by reflected particles incident from the left or from the right.

Thouless [28] has shown the existence of a dispersion relation between the localization length and the DOS. This relationship can be expressed [29] in the form of a linear dispersion relation between the real, $\mathrm{Re}\ln t$, and imaginary, $\mathrm{Im}\ln t$, parts of the complex transmission amplitude. Similar relations also hold between the partial DOS and the sensitivity [22]. As the self-averaging properties of $\tau_{z,T}^{\mathrm{BL}}$ and of $\tau_{y,T}^{\mathrm{BL}}$ in disordered systems they are an immediate consequence of self-averaging of the localization length and of the DOS [29]. It means, that $\tau_{y,T}$ is additive, in the sense that

$$\tau_{y,T}^{\mathrm{BL}}(0, L) = \mathrm{Im}\int_0^L G(y, y)\,dy = \tau_{y,T}^{\mathrm{BL}}(0, y) + \tau_{y,T}^{\mathrm{BL}}(y, L) \tag{2.23}$$

as we can easily deduce from eqns (2.19). A similar relation holds for the $\tau_{z,T}^{\mathrm{BL}}$ too. This property has been pointed out by Leavens and Aers [25] when they discussed the local version of the Larmor clock with an arbitrary barrier potential and a localized magnetic field inside the barrier.

2.2. Reflection time

It is clear that the orientation of the spin of the reflected wave and so the BL reflection time τ_R^{BL} from the arbitrary 1D barrier can be calculated in the same way as we have done for the transmitted wave (see eqns (2.9)–(2.18)). Proceeding as above, we find

$$\begin{aligned}\langle S_z\rangle_R &= \tfrac{1}{2}\langle(\Psi(0)-1)|\sigma_z|(\Psi(0)-1)\rangle \\ &= 4B\,\mathrm{Re}(\psi^*(0)-1)\int_0^L \psi(y)G(0, y)\,dy \end{aligned}\tag{2.24}$$

$$\langle S_y\rangle_R = -4B\,\mathrm{Im}(\psi^*(0)-1)\int_0^L \psi(y)G(0, y)\,dy \tag{2.25}$$

$$\langle S_x\rangle_R = 2|\psi^*(0)-1|^2\left(1 - B^2\left|\int_0^L \psi(y)G(0, y)\,dy\right|^2\right) \tag{2.26}$$

and finally:

$$\tau_{y,R}^{\mathrm{BL}} = \mathrm{Im}\,\frac{1+r}{r}e^{-2i\theta(0)}\int_0^L G(y,y)e^{2i\theta(y)}\,dy$$
$$= \mathrm{Im}\,\frac{1}{2k}\left\{\frac{\partial \ln r}{\partial k} - \frac{1}{2kr}(1-r^2-t^2)\right\} \tag{2.27}$$
$$\tau_{z,R}^{\mathrm{BL}} = \mathrm{Re}\,\frac{1+r}{r}e^{-2i\theta(0)}\int_0^L G(y,y)e^{2i\theta(y)}\,dy$$
$$= \mathrm{Re}\,\frac{1}{2k}\left\{\frac{\partial \ln r}{\partial k} - \frac{1}{2kr}(1-r^2-t^2)\right\} \tag{2.28}$$

where $\theta(y)$ is given by eqn (2.12).

These expressions are the main results of this paper and are valid for an arbitrary 1D potential shape $V(y)$. Together with the eqns (2.19) and (2.20) they complete the set of BL times in terms of the scattering-matrix elements. Note that the second term in eqns (2.27) and (2.28) is of the same order of magnitude as the analogous one in eqns (2.19) and (2.20) and so becomes important for an open and finite system.

Some of the well-known relations between the components $\tau_{y,T}^{\mathrm{BL}}$, $\tau_{z,T}^{\mathrm{BL}}$, $\tau_{y,R}^{\mathrm{BL}}$ and $\tau_{z,R}^{\mathrm{BL}}$ (see [1]) can be checked directly, using the explicit expressions (2.19), (2.20), (2.27) and (2.28). Indeed for an arbitrary symmetric barrier, where $r = r'$, i.e. the total phase accumulated in a transmission and reflection event is the same ($\varphi_a \equiv 0$), one has therefore

$$\tau_{y,T}^{\mathrm{BL}} = \tau_{y,R}^{\mathrm{BL}}. \tag{2.29}$$

For the special case of a rectangular barrier, eqn (2.29) was found first by Büttiker [8]. Comparison of eqns (2.19) and (2.27) show that for asymmetric barrier eqn (2.29) breaks down [16].

Another identity, as an equation of conservation of angular momentum [8, 10]

$$R\tau_{z,R}^{\mathrm{BL}} + T\tau_{z,T}^{\mathrm{BL}} = 0$$

immediately follows from eqns (2.20) and (2.28).

Finally the dwell time τ^{D} [8, 10, 25, 1] can be written as

$$\tau_{-}^{\mathrm{D}} \equiv T\tau_{y,T}^{\mathrm{BL}} + R\tau_{y,R}^{\mathrm{BL}} = \frac{1}{2k}\,\mathrm{Im}\left\{\frac{\partial \ln t}{\partial k} + \frac{1}{2k}(r+r')\right\} + \frac{R}{2k}\,\mathrm{Im}\left\{\left(\frac{\partial \ln r}{\partial k} - \frac{\partial \ln t}{\partial k}\right) - \frac{1}{2kr}(1+rr'-t^2)\right\}. \tag{2.30}$$

The subscript minus indicates that the particle is coming from the left. A similar expression to (2.30) was obtained in [30] and holds when the particle is coming from the right, interchanging r and r'.

2.3. Escape of an electron from a finite disordered region

It should be clear that the concepts of the surface GF method discussed in this article, apply not only to the traversal time of tunneling but can be generalized to the escape problem of the electron from the 1D disordered region. To show this, we consider the case where an arbitrary and finite 1D barrier potential break up into two, left ($0 < y < y_0$) and right ($y_0 < y < L$) blocks. We shall assume that the electron with the initial coordinate $y = y_0$ escapes from the region when it reaches one end of the system: $y_0 = 0$ or $y = L$. To calculate, for example, the escape time $\tau_r^{\mathrm{esc}}(y_0, L; E_0)$ on the right-hand side of the disordered region we will use the local version of Larmor clock [26], where Büttiker's analysis [9] was extended to the local situation in which a uniform transverse magnetic field is confined to an arbitrary part of a barrier. It means that in our case $\boldsymbol{B}$ is finite only in the interval $[y_0, L]$. Along the lines of Section 2 one derives (see Appendix B)

$$\tau_{r,y}^{\mathrm{esc}}(y_0, L; E) = \mathrm{Im}\int_{y_0}^{L} G(y,y;E)\,dy$$

$$\tau^{\mathrm{esc}}_{r,y}(y_0, L; E) = \mathrm{Im}\int_{y_0}^{L} G(y, y; E)\, dy$$
$$= \mathrm{Im}\left\{\frac{\partial \ln t_r}{\partial E} + \frac{1}{4E}(\tilde{r}_r + r') + \frac{1}{2}(1-\tilde{r}_r)\frac{\partial}{\partial E}\ln\frac{1-\tilde{r}_r}{1+\tilde{r}_e}\right\}, \qquad (2.31)$$

$t_r(y_0, L; E)$ is the complex amplitude of transmission only through the right block and r' is the reflection amplitude of the electron from the whole system, when it falls in from the right (see eqns (2.19), (2.20)). $\tilde{r}_r \equiv \tilde{r}_r(y_0, L; E)(\tilde{r}_e \equiv \tilde{r}_e(y_0, L; E))$ has slightly different meaning: the tilde mark signifies that the given quantity is calculated in the presence of the left and right blocks [20]. Thus $\tilde{r}_r(\tilde{r}_e)$ is the complex amplitude of reflection from the right (left) block in the presence of the left (right) block, when the electron falls in this block from the left (right). Analogous expressions hold for the second component of escape-time $\tau^{\mathrm{esc}}_{r,y}(y_0, L; E) = \mathrm{Re}\int_{y_0}^{L} G(y, y; E)\, dy$ and for the particle, escaping on the left-hand side of the disordered region.

For $y_0 = 0$ the eqn (2.31) coincides obviously with eqn (2.19), i.e., with the problem of the free incidence of the electron from the left on the 1D arbitrary potential. We have thus arrived at a sample relationship between the two components of escape time of an electron from a finite disordered region and the *local scattering-matrix elements*. It is seen from eqns (2.31), that the time required by an electron to cover a distance L in the disordered region is extremely sensitive to the boundary conditions and on its initial position y_0. With respect to the chemical nanostructures mentioned in the Introduction, escape time out of a quantum well can have different orders of magnitude [31]. Note that expression (2.31) is valid not only for the escape of the electron but also for any other times, e.g. the lifetime, characterizing the behavior of an electron within a given potential shape [32].

3. Conclusions

To conclude, one would like to stress that the surface GF method, which is not a perturbation approach, is very appropriate for practical calculations of the transmission, reflection and dwell times for an arbitrary barrier potential. Three characteristic times, as well as the escape time of an electron from a finite disordered region were expressed in terms of the scattering-matrix elements.

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Appendix A. Basic concept of surface Green's function

To calculate the τ_T^{BL} traversal time, defined by eqn (2.18), we follow closely [20] and introduce the following general model. Let us consider that our system can be divided into $(N-1)$ layers, labelled $n = \{1, \ldots, N-1\}$, which are placed between two semi-infinite media. The positions of the boundaries of the nth layer are given by y_n and y_{n+1}. We allow a possible discontinuity in the potential $V_n(y)$ at each boundary between two layers. Let us assume that a plane wave is incident from the left onto the boundary $y = y_1$ and evaluate the amplitude of the reflected wave and the wave propagating in the semi-infinite media for $y \geq y_N$. For this purpose we will use the surface GF method, as mentioned in the Introduction. 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.

Let us first discuss the contact of two semi-infinite media; this will clearly show the spirit of the method. Assume that the potential energy of the electron is $V_0(y)$ on the left of the boundary at $y_1(y < y_1)$ and $V_1(y)$

on the right at y_1 and that 1D electron GF $G_n^{(0)}(y, y'; E)(n = 0, 1)$ for each medium are known, when the corresponding media are infinite. The following equation holds:

$$\left[-\frac{\partial^2}{\partial y^2} + V_n(y) - E\right] G_n^{(0)}(y, y'; E) = \delta(y - y'). \tag{A1}$$

We shall consider below constant potentials V_n with arbitrary strength for two cases when we have free electrons or an additional external homogeneous electrical field present ($V_{\text{ext}} = V_n + Fy$). The upper index (l) of GF (in eqn (A1) the index $l = 0$) will indicate the number of boundaries considered in the calculation of a given GF. The lower index of the GF labels the interval for which the GF is valid. The GF on the left of the boundary $(y, y' \leq y_1)$ is given by [20]:

$$G_0^{(1)}(y, y') = G_0^{(0)}(y, y') + r_{01}\frac{G_0^{(0)}(y, y')G_0^{(0)}(y_1, y')}{G_0^{(0)}(y_1, y_1)}, \tag{A2}$$

where r_{01} is the amplitude of the reflection of the electron propagating from region 0 into 1. The first term on the right-hand side corresponds to direct propagation and the second term to reflection on the surface. A similar expression holds in the region on the left of the boundary. The continuity of the GF and the equality of currents at the boundary $y = y_1$ allow us to calculate the two amplitudes of reflection coefficients r_{01} and r_{10} (from region 1 into 0) ($G_n^{(0)} \equiv G_n^{(0)}(y_1, y_1), n = 0, 1$):

$$r_{10} = -r_{01} = \frac{G_0^{(0)} - G_1^{(0)}}{G_0^{(0)} + G_1^{(0)}}. \tag{A3}$$

Adding new boundaries and each time using the previously obtained GF as the starting point we derive the new amplitude of reflection of the electron. Finally, the GF for the complete system at coinciding coordinates in the nth layer (the left block containing n boundaries and a right block consisting of $(N - n)$ boundaries) is given by:

$$G_n^{(N)}(y, y) = \frac{G_n^{(0)}(y, y)}{D_N}\left[1 + R_{n,n-1}^{(n)}R_{n,n+1}^{(-n+N)}\lambda_{n,n+1} + R_{n,n-1}^{(n)}e^{2i[\theta_n(y)-\theta_n(y_n)]} + R_{n,n+1}^{(-n+N)}e^{2i[\theta_n(y_{n+1})-\theta_n(y)]}\right]. \tag{A4}$$

Here D_N is a characteristic determinant (or denominator of the whole system GF) and can be expressed as the product:

$$D_N = D_N^0\left\{\prod_{n=1}^{N}\lambda_{n-1,n}(1 + r_{n,n-1})(1 + r_{n-1,n})\right\}^{-1/2}. \tag{A5}$$

The factors $\lambda_{n-1,n}$ are defined, in general, as

$$\lambda_{n-1,n} = \exp\left(-\int_{y_{n-1}}^{y_n}\frac{dy}{G_{n-1}^{(0)}(y, y)}\right), \tag{A6}$$

and 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 $n - 1$) and can be obtained from eqn (A3) by replacing in the lower indices $0 \to n - 1$, $1 \to n$ and $y_1 \to y_n$. The complex quantity $R_{n,n-1}^{(n)}$ in eqn (A4) is the amplitude of reflection from the left block, containing n boundaries (when the electron falls on this block from the right), and $R_{n,n+1}^{(-n+N)}$ is the amplitude of reflection from the right block, containing $N - n$ boundaries (when the electron falls on this block from the left) [20].

To conclude this appendix let us note that the GF on the right side of the Nth boundary $(y, y' \geq y_N)$ has

the following form:

$$G_N^{(N)}(y, y') = G_N^{(0)}(y, y') + R_{N,N-1}^{(N)} \frac{G_N^{(0)}(y, y_N) G_N^{(0)}(y_N, y')}{G_N^{(0)}(y_N, y_N)}. \tag{A7}$$

Here $R_{N,N-1}^{(N)}$ is the reflection amplitude of the whole system from the Nth boundary when the electron falls in from the right.

In a similar way, the GF on the left of the system ($y, y' \leq y_1$) can be written as:

$$G_0^{(N)}(y, y') = G_0^{(0)}(y, y') + R_{0,1}^{(N)} \frac{G_0^{(0)}(y, y_1) G_0^{(0)}(y_1, y')}{G_0^{(0)}(y_1, y_1)} \tag{A8}$$

where $R_{0,1}^{(N)}$ is the reflection amplitude of the system from the first boundary when the wave falls in from the left.

With this brief introduction to the surface GF method, we are ready to calculate the coefficient of transmission through a 1D random-layered system. By means of the definition, the coefficient of transparency through a multilayered structure is expressed as the square amplitude of the wavefunction from the right (if the electron falls in from the left) of the given structure and it may be written, using the Fisher–Lee relation between the scattering matrix and the GF [33]

$$T = [|G_0^{(0)}(y_1, y_1) \| G_N^{(0)}(y_N, y_N)|]^{-1} |G^N(y_1, y_N)|^2 \tag{A9}$$

where $G^N(y_1, y_N)$ is the GF of the electron in the layered structure with N boundaries.

Using the relation (2.11) for general expression of the $G(y, y')$ in terms of coinciding coordinates $y = y'$ we can write:

$$G^{(N)}(y_1, y_N) = [|G^{(N)}(y_1, y_1) \| G^{(N)}(y_N, y_N)|]^{1/2} \exp i[\theta(y_N) - \theta(y_1)]. \tag{A10}$$

Where

$$i\theta(y_N) - \theta(y_1) = -\int_{y_1}^{y_N} \frac{dy}{2G^{(N)}(y, y)} = -\sum_{n=1}^{N-1} \int_{y_n}^{y_{n+1}} \frac{dy}{2G_n^{(N)}(y, y)}. \tag{A11}$$

Here $G_n^{(N)}(y, y)$, $G_N^{(N)}(y, y')$ and $G_0^{(N)}(y, y')$ are defined by eqns (A4), (A7) and (A8) respectively.

To calculate the integral appearing in eqn (A11) we shall make use of eqn (2.12), the connected phase function $\theta(y, E)$ and the GF, as well as eqn (A4) for $G_n^{(N)}(y, y)$:

$$-\int_{y_n}^{y_{n+1}} \frac{dy}{2G_n^{(N)}(y, y)} = \frac{1}{2} \ln \frac{\lambda_{n,n+1}(1 + R_{n,n-1}^{(n)})(1 + R_{n,n+1}^{(-n+N)})}{(1 + \lambda_{n,n-1} R_{n,n+1}^{(n)})(1 + \lambda_{n,n+1} R_{n,n+1}^{(-n+N)})}. \tag{A12}$$

In view of eqn (A12) let us present eqn (A10) in its final form:

$$G^{(N)}(y_1, y_N) = (D_N^0)^{-1} \left(G_0^{(0)}(y_1, y_1) G_N^{(0)}(y_N, y_N) \prod_{n=1}^{N-1} (1 + r_{n,n-1})(1 + r_{n-1,n}) \right)^{1/2}. \tag{A13}$$

Substituting eqn (A13) into eqn (A9) for the GF $G^{(N)}(y_1, y_N)$ and using the analogous expression for $[G^{(N)}(y_1, y_N)]^*$ we can finally show that the coefficient of transmission through a multilayered structure is inversely proportional to the characteristic determinant D_N:

$$T = |D_N|^{-2} \tag{A14}$$

where D_N is given by (A5).

Appendix B. Integral of the Green's function

First, we can trivially rewrite the wavefunction $\psi(y)$, which is a solution of the Schrödinger equation, as:

$$\psi(y) = [V(y) - E]\frac{\partial}{\partial E}\psi(y) - \frac{\partial}{\partial E}[V(y) - E]\psi(y). \tag{B1}$$

Hence, the square of the wavefunction can be rewritten in the form

$$\psi(y)^2 = \psi''(y)\frac{\partial}{\partial E}\psi(y) - \psi(y)\frac{\partial}{\partial E}\psi''(y) \equiv \frac{\partial}{\partial y}\left[\psi'(y)\frac{\partial}{\partial E}\psi(y) - \psi(y)\frac{\partial}{\partial E}\psi'(y)\right]. \tag{B2}$$

Integrating both parts of this expression over y one gets

$$\int \psi(y)^2\, dy = -\psi(y)^2\frac{\partial}{\partial E}\left(\frac{\psi'}{\psi}\right) \equiv -\psi(y)^2\frac{\partial}{\partial E}\left(\frac{\psi'\psi^*}{|\psi|^2}\right). \tag{B3}$$

Substituting the wavefunction in the form

$$\psi = |\psi|e^{i\theta} \tag{B4}$$

one can write (B3) in the following form:

$$\int G(y, y)e^{2i\theta(y,E)}\, dy = -\frac{G(y, y)}{2}e^{2i\theta(y)}\frac{\partial}{\partial E}\left[\frac{G'(y, y) - 1}{G(y, y)}\right]. \tag{B5}$$

In a similar way, one has:

$$\int G(y, y)e^{-2i\theta(y,E)}\, dy = -\frac{G(y, y)}{2}e^{-2i\theta(y)}\frac{\partial}{\partial E}\left[\frac{G'(y, y) + 1}{G(y, y)}\right]. \tag{B6}$$

We derived eqns (B5) and (B6) making use of the fact that the wavefunction $\psi(y)$ at energy E is related to the retarded GF $G(y, y')$ of the system through the expression:

$$G(y, y') = \begin{cases} i\pi\nu_L(E)\psi(y)\psi^*(y') & \text{if } x > x' \\ i\pi\nu_L(E)\psi^*(y)\psi(y') & \text{if } x \le x' \end{cases} \tag{B7}$$

where $\nu_L(E)$ is the DOS per unit energy and per unit length. Note that at coinciding coordinates, this expression reduces to the well-known result $G(y, y) = i\pi\nu_L(E)|\psi(y)|^2$.

Using the expressions (B1) and (B2) we can present $|\psi(y)|^2$ in the following form

$$|\psi(y)|^2 = \frac{1}{2}\frac{\partial}{\partial y}\left\{\left[\psi'(y)\frac{\partial}{\partial E}\psi^*(y) + \psi^{*'}(y)\frac{\partial}{\partial E}\psi(y)\right] - \left[\psi(y)\frac{\partial}{\partial E}\psi^{*'}(y) + \psi^*(y)\frac{\partial}{\partial E}\psi'(y)\right]\right\}. \tag{B8}$$

Integrating both parts of the modulus square $|\psi(y)|^2$ over y one shows

$$\int |\psi(y)|^2\, dy = -\frac{1}{2}\left\{\psi^{*2}(y)\frac{\partial}{\partial E}\left[\frac{\psi'(y)\psi(y)}{|\psi(y)|^2}\right] + \psi^2(y)\frac{\partial}{\partial E}\left[\frac{\psi^{*'}(y)\psi^*(y)}{|\psi(y)|^2}\right]\right\}. \tag{B9}$$

The straightforward calculation, using eqns (B4) and (B7) leads to

$$\int G(y, y)\, dy = i\frac{\partial}{\partial E}\theta(y; E) - \frac{G(y, y)}{2}\frac{\partial}{\partial E}\left[\frac{G'(y, y)}{G(y, y)}\right]. \tag{B10}$$

This completes the set of useful integrals which were used in this article.

Now we can go a step further and calculate the integral (B10) in the given region $[0, L]$ in order to calculate the τ_T traversal time, defined by eqn (2.18). Without loss of generality we will discuss the case when the barrier potential $V(y)$ is zero outside the interval $[0, L]$, i.e. $G_0^{(0)}(0, 0) = G_N^{(0)}(L, L) = i/2k$.

Note that the expressions relating reflection amplitudes to the GF (A7) and (A8) can be read as ($r \equiv R_{0,1}^{(N)}$ and $r' \equiv R_{N,N-1}^{(N)}$)

$$G(0,0) = G_0(0,0)(1+r) \tag{B11}$$

$$G(L,L) = G_0(0,0)(1+r'). \tag{B12}$$

As for the derivatives $G'(y,y)$ at 0 and L we have respectively

$$G'(0,0) = r \tag{B13}$$

$$G'(L,L) = -r'. \tag{B14}$$

Making use of eqns (B11)–(B14) we can rewrite the integral (B10) as

$$\int_0^L G(y,y;E)\,dy = i\frac{\partial}{\partial E}[\theta(L;E) - \theta(0;E)] + \frac{\partial}{\partial E}\ln(1+r)(1+r') + \frac{1}{4E}(r+r'). \tag{B15}$$

The next step to get the final answer is to calculate the first bracket in eqn (B15). It is straightforward to show, using eqns (A12) and (A13) that the bracket can be presented in the form:

$$i[\theta(L;E) - \theta(0;E)] = \ln\frac{t}{(1+r)(1+r')}.$$

This completes the proof: substituting into eqn (B15) we finally obtain the τ_T^{BL} traversal time (2.18).

In the rest of this appendix we present the explicit expressions for the integral of $G_n^{(N)}(y,y)$ given by eqn (A4) in each layer and show that the sum of all the contributions of all layers correspond to the results of [10, 16, 17]. For a piece-wise constant potential, as was done by Aronov *et al.* [20] the result is:

$$\int_{y_n}^{y_{n+1}} G_n^{(N)}(y,y)\,dy = \frac{\partial \ln t}{\partial V_n}, \tag{B16}$$

where V_n is the potential energy of electron in the nth subsystem and t is the complex amplitude of the transmission between 0 and L. We could write the total integral of the eqn (B16) in the form:

$$\int_0^L G^{(N)}(y,y)\,dy = \sum_{n=1}^{N-1}\int_{y_n}^{y_{n+1}} G_n^{(N)}(y,y)\,dy = \sum_{n=1}^{N-1}\frac{\partial \ln t}{\partial V_n}. \tag{B17}$$

In the $N \to \infty$ limit (keeping L fixed) and converting the summation into an integral the eqn (B17) can be written

$$\int_0^L G(y,y)\,dy = \int_0^L \frac{\delta \ln t(y)}{\delta V(y)}\,dy, \tag{B18}$$

where $\delta/\delta V(y)$ is a functional derivative: this is the result of Sokolovski and Baskin [10]. On the other hand, as was shown in [16], the functional derivative with respect to the potential can be replaced by the derivative with respect to the average height of the potential $\bar{V}$ (keeping the spatial variation of the potential fixed). It means that

$$\int_0^L \frac{\delta \ln t(y)}{\delta V(y)}\,dy = \frac{\delta \ln t}{\delta \bar{V}} \tag{B19}$$

and so

$$\frac{\delta \ln t}{\delta \bar{V}} = \int_0^L G(y,y)\,dy = \frac{\partial}{\partial E}\ln t + \frac{1}{4E}(r+r') \tag{B20}$$

as we might expect.

In the time-modulated barrier approach of Büttiker and Landauer [7, 13], where the original static V_0 barrier

was augmented by a small oscillation in the barrier height, e.g. $V_1 \cos \varpi t$ (ϖ is the modulation frequency and $\varpi \ll V_1$), it was shown that for an opaque barrier $\chi L \gg 1 (\chi = \sqrt{V_0 - E})$ can be defined as an asymmetry function which was characterized by a single quantity with the dimension of time

$$\tau_T = L/2\chi. \tag{B21}$$

The time τ_T separates characteristic low- and high-frequency behaviors and can be identified with the traversal time for tunneling. On the other hand using the basic idea of [8, 14], Jahou and Jonson [18] showed that in the adiabatic $\varpi \to 0$ limit and for an arbitrary-shaped potential barrier the traversal time τ_T (B21) must be replaced formally by the modulus of the complex quantity

$$\tau_T^{\bar{V}} = i \frac{\partial \ln t(E, \bar{V})}{\partial \bar{V}} \tag{B22}$$

which is closely related to the complex times introduced in [10, 16, 25]. But as shown above (see eqn (B20)) eqn (B22) is equivalent to eqns (2.19) and (2.20), because the derivative with respect to the average height of the potential can be presented in terms of partial derivatives with respect to energy E [12]. Thus we show that most results, obtained from very different points of view [10, 16, 17], are almost compatible and the final results can be expressed in terms of the GF and the scattering-matrix elements.

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