

Landauer formula for transmission across an interface

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We reconsider the classical problem of the quantum-mechanical resistance due to a quantum-mechanical reflection off a heterostructure interface. In the presence of a current, the electron distribution in the vicinity of the interface is different from that in the bulk due to the angular dependence of the reflection coefficient. The interface also modifies the electron concentration, leading to a violation of the local neutrality. This creates a self-consistent electric field and affects the angular distribution. The interface resistance depends on the actual form of the electron distribution. Incorporating all these factors in a kinetic transport model, we have reduced evaluation of the resistance to an integral equation. The equation is solved analytically in the limits of either strong or weak reflection. A simple model shows an appreciable difference between our results and the conventional Landauer approach.

I. INTRODUCTION

The Landauer resistance formula has been very helpful in describing mesoscopic devices where only a few scatterers are active and the resulting resistance is conveniently described by a scattering matrix. This approach is very different from that employed in calculations of the resistivity of a medium with many random scatterers (e.g., impurities or phonons). That approach, usually involving an average with respect to various possible arrangements of the scatterers, cannot be applied to the case of a small number of scatterers.

It is also attractive to use the Landauer formula in heterostructure-interface-transmission problems. Indeed, a planar interface can be characterized by the transmission and reflection coefficients and one is naturally tempted to express the interface resistance in terms of these coefficients. Such an expression was originally obtained by Landauer.¹ Assuming the zero-temperature Fermi distribution for electrons, he derived the following formula for the conductance per unit area of a planar scatterer:

$$G = \frac{e^2 k^2}{8\pi^3 \hbar} \int \frac{1 - R(\cos \theta)}{R(\cos \theta)} |\cos \theta| d\Omega, \quad (1)$$

where $R(\cos \theta)$ is the reflection coefficient depending on the electron incident angle θ and k is the Fermi wave vector.

In the subsequent discussion Landauer considered the possibility that the electron distribution function was modified due to an interference between the scattering plane and the thermal scattering, leading to a deviation from Eq. (1). Landauer stated¹ that such a deviation would imply a violation of Matthiessen's rule for resistivities.

Precisely this situation takes place in heterostructure devices. The distance between the interface and the leads is often much larger than the electron mean free path. The distribution of electrons incident to the interface is formed by elastic scattering far from it. Near the interface this distribution is changed for two reasons. First, the distribution is affected by the angular dependence of the reflection and transmission coefficients. Second, an electric current across the interface leads to a violation of local neutrality. Due to reflections, the electron concentration is higher on the side of the incoming flux and lower on the other side. The resulting self-consistent field affects the electron distribution function. The latter effect is linear in the electric field and contributes to the Ohmic resistance.^{1,2} Therefore the Landauer formula, in which the reflection and transmission coefficients of an interface are independent of any scattering in its vicinity, cannot be used in devices of the length larger than the electron mean free path. It needs some modification. Such a modification can be considered as the calculation of effective reflection and transmission coefficients taking into account scattering in the vicinity of the interface.

The purpose of the present paper is to discuss the necessary modification of Landauer's formula. As an example, we calculate the resistance of a planar potential barrier, similar to that in a GaAs/Al_xGa_{1-x}As/GaAs heterostructure. In this case calculations are a bit simpler because the effective masses and electron affinities on both sides of the interface are equal. For the one-dimensional case, such a problem has been studied by Eränen and Sinkkonen.³

The interface resistance problem has some similarity to a multichannel mesoscopic device. There are several definitions of the multichannel device resistance which lead to different results (see Refs. 4-6 and references therein). In a degenerate electron gas only the angular distribution

of incident electrons is of importance and a small solid angle can be regarded as one channel. It is impossible, however, to make a direct use of the multichannel Landauer formulas for the calculation of the interface resistance, because of rather strong limitations under which these formulas are derived. The most important limitation is the assumption of no exchange of electrons between different channels. Also, the electron concentrations in both incoming and outgoing channels are determined by the corresponding reservoirs and the coefficients of reflection and transmission (see Refs. 4–6 and references therein). Neither of these conditions is satisfied for a heterostructure interface. Far away from the interface, the nonequilibrium part of the distribution function is determined by an interplay between the electric field and the scattering. Within a mean free path from the interface, the distribution is modified by the transmission and reflection. The angular distribution near the interface is influenced by all these factors.

The same problem can be viewed from another point. All previous derivations of the Landauer formula have used balance equations and described deviations from equilibrium by a shift in the chemical potential. Such an approach is justified for the degenerate gas in a one-dimensional (1D) channel, where electronic states participating in the transport are characterized only by the sign of the velocity. In this language, channels corresponding to different incoming and outgoing angles in the interface problem must be characterized by different chemical potentials, whose angular dependence remains to be determined.

In the context of ballistic devices, the Landauer formula describes the resistance of an interface or a constriction separating two thermal baths with different electrochemical potentials. The resistance is defined as the ratio of the electrochemical potential difference to the current. There is, however, a problem of the definition of the potential difference in a ballistic device.^{7,4,8,5} Such a problem does not exist in our case where the dimensions of both the device and the contacts are much larger than the electron mean free path.

In the next section, we specify our definition of the barrier resistance. This definition, in principle, can be used also for ballistic devices; in order to illustrate its physical meaning, we apply it to a well-studied example of the multichannel Landauer formula for a ballistic device.

The structure which is of main interest for us is an interface separating two semiconductors with the size larger than the electron mean free path. Such a structure is nonuniform and the resistance of its different parts is usually calculated with different approaches. For the calculation of the interface resistance in a ballistic device a quantum-mechanical calculation of the transmission and reflection coefficients is necessary. The resistivity of a uniform medium, in the case of a weak scattering, is calculated with the help of the Boltzmann equation. For a structure consisting of an interface imbedded in a resistive medium, it is necessary to combine both of these approaches. The interface can be characterized by reflection and transmission coefficients obtained from a quantum-mechanical calculation. In such a calculation the asymptotic

of the electron wave function far from the interface are plane waves. We assume that the electron mean free path l is much larger than the de Broglie wavelength λ . In this case the transmission and reflection coefficients can be used to write down the boundary conditions connecting the electron distribution function at opposite sides of the interface. In principle, these coefficients can incorporate also interface roughness and underbarrier impurity scattering. The condition $\lambda \ll l$ also justifies the classical Boltzmann equation.

Being transmitted through (or reflected by) the interface, an electron is scattered by impurities. The size of the structure L is assumed to be much larger than the mean free path, so that the number of impurities which have a chance to scatter an electron before it reaches a lead or comes back to the interface is very large. That means that there are regions far from the interface which are characterized by a uniform electric field controlled by a total current. In the regions of the semiconductors close to the interface the electric field deviates from its constant value far from the interface and the electron distribution function is formed under the effect of both interface transmission-reflection and collisions. The redistribution of the electric field near a small constriction has been studied for mesoscopic devices where both classical and quantum approaches have been used.^{9–11} Such a redistribution is important in the analysis of resonant-tunneling diodes.¹² Technically our approach is different from the previous ones because we consider the case of elastic scattering and neglect any energy relaxation, which is possible for the calculation of the resistance in the Ohmic region. In earlier works (see, e.g., Ref. 9) a form of the collision operator was used which does not distinguish between the energy and momentum relaxation.

A problem very similar to ours was studied by Zaitseva and Levinson.¹³ They looked for boundary conditions for the thermoconductivity equation at the interface between two materials. For this purpose they solved the Boltzmann equation for phonons at the presence of a temperature gradient in the region about the phonon mean free path near the interface. Zaitseva and Levinson used reflection and transmission coefficients to connect the phonon distribution function at different sides of the interface. Far from the interface, the angle-averaged distribution function satisfied the diffusion equation and in the vicinity of the interface it is distorted by the angular dependence of the reflection and transmission coefficients.

In Sec. III we solve the Boltzmann equation for a simple model of a resistive medium separated into two parts by a flat potential barrier. Our approach can be generalized to the case when the effective masses or electron affinities on opposite sides of the interface are different, but this case is not discussed here. We consider only the case of a degenerate electron gas; this simplifies the problem by removing from consideration any particular energy dependence of the relaxation time. The problem is reduced to an integral equation for a local electrochemical potential. An analytic solution to this equation and an explicit formula for the resistance of the barrier are obtained for a strong and a weak reflection in Secs. IV

and V , respectively. In Sec. VI we make a simple model calculation and compare our result with Eq. (1).

II. DEFINITION OF THE INTERFACE RESISTANCE

This definition is nontrivial because an interface not only contributes a resistance due to its reflectivity but also changes the resistance of nearby regions of the sample. Physically, these effects cannot be separated. As shown in the next section, the presence of a barrier changes the electron distribution and the electric field within a region of about one electronic mean free path from the barrier. It makes sense to include this region with the barrier in one unit, whose resistance (henceforth referred to as the barrier resistance) is then operationally defined as the difference between the resistance of two heterostructures identical in every respect, except for the barrier present in one structure and absent in the other. This contribution to the resistivity satisfies Matthiessen's rule in the sense that it does not interfere with contributions resulting from scattering outside the barrier region.

Such a definition can be generalized for an interface between different materials. One can assume that a heterostructure with a nonresistive interface consists of two materials with a uniform electric field in each of them and a continuous electric potential at the interface. The resistance of such a structure is the sum of the resistances of each of the materials. In a real structure the electric field near the interface is nonuniform. The extrapolation of the uniform potential distribution from the regions far from the interface shows that the nonuniform distribution of the potential is equivalent to a discontinuity of the electric potential at the interface. The resistance of the interface can be defined as the ratio of this potential discontinuity to the electric current.

Our definition of the resistance is convenient practically for the case of vertical transport in heterostructures because it allows us to add other resistances in series. For other measurement arrangements, e.g., for four-probe measurements, the definition of the resistance may be different.

To illustrate the above definition we apply it to a well-studied case of a mesoscopic device consisting of two reservoirs connected by N identical 1D channels (Fig. 1). The device in Fig. 1(b) is different from that in Fig. 1(a) by the presence of a scatterer, which induces interchannel transitions described with the coefficients of transmission T_{ab} and reflection R_{ab} . For simplicity, we assume that these coefficients are symmetric with respect to the direction of propagation. We consider zero temperature and assume that the difference between chemical potentials of the reservoirs is small, $\Delta\mu = \mu_L - \mu_R$, where μ_L and μ_R refer, respectively, to the left and the right reservoirs.

For the device in Fig. 1(a), it is evident that electrons below μ_R do not contribute to the electric current because their oppositely directed fluxes cancel each other in each channel at any energy below μ_R . Due to the unitarity relation¹⁴

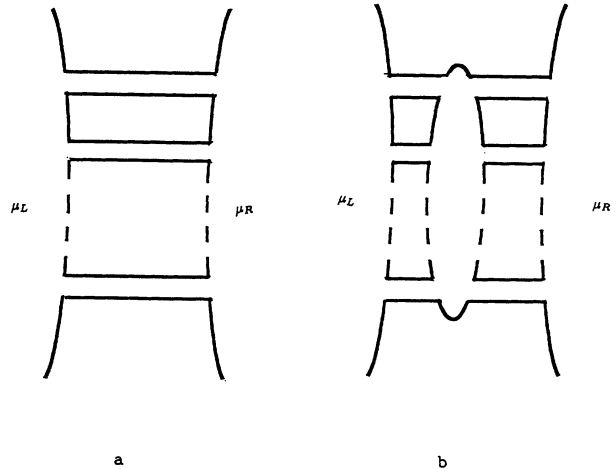


FIG. 1. Two devices consisting of two thermal baths with electrochemical potentials μ_L and μ_R , respectively, connected by conducting channels. The devices are identical in all respects except that in device (a) there is no scattering between the channels and device (b) contains a scatterer. The resistance of the scatterer is defined as a difference between the resistance of the device with the scatterer (a) and that of the device without the scatterer (b).

$$\sum_b (R_{ab} + T_{ab}) = 1, \quad (2)$$

the same situation takes place in the device in Fig. 1(b).

This means that the conductance is entirely determined by the current of electrons in the energy interval between μ_R and μ_L . An electron emerging from any channel on either side is scattered many times in the corresponding reservoir before returning to the same or a different channel. Therefore, electrons entering each channel are in equilibrium with the reservoir and the net flux is from left to right in each channel between μ_R and μ_L . The current in the a th channel is given by

$$j_a = \frac{e}{\pi\hbar} \sum_b (1 - R_{ab}) = \frac{e}{\pi\hbar} \sum_b T_{ab}, \quad (3)$$

where the total conductance is

$$G_0 = \frac{e^2}{\pi\hbar} N, \quad (4)$$

for the device in Fig. 1(a) and

$$G = \frac{e^2}{\pi\hbar} \mathcal{T}, \quad \mathcal{T} = \sum_{ab} T_{ab}, \quad (5)$$

for the device in Fig. 1(b). Our definition of the resistance \mathcal{R} associated with the scatterer, corresponds to

$$\mathcal{R} = \frac{\pi\hbar}{e^2} \frac{N - \mathcal{T}}{N\mathcal{T}}. \quad (6)$$

This expression with some assumptions was first obtained

by Langreth and Abrahams.¹⁴ Equation (4) corresponds to the resistance of N channels without any scattering, usually referred to as the contact resistance. The total resistance of the device in Fig. 1(b) is the sum of the contact resistance and the resistance of the inserted scatterer.

III. GENERAL EXPRESSION FOR THE RESISTANCE OF A BARRIER

Our calculation of the resistance of a heterostructure containing a barrier will be based on the Boltzmann equation, commonly used in the description of transport in a continuous medium. We consider the 3D case with a single planar symmetric barrier similar to that in GaAs/Al_xGa_{1-x}As/GaAs heterostructures, and neglect any scattering by surface roughness or by impurities under the barrier.

We assume that the elastic relaxation time τ resulting from electron-impurity scattering is much shorter than the inelastic relaxation time. On each side of the barrier, the Boltzmann equation is of the form

$$v_z \frac{\partial f}{\partial z} + eF \frac{\partial f}{\partial p_z} = \frac{\bar{f} - f}{\tau}, \quad (7)$$

where v_z and p_z are the z components of the electron velocity and momentum, $F(z)$ is the electric field, and \bar{f} is the angular average value of the electron distribution function $f(\mathbf{p})$, viz.,

$$\bar{f}(z) = \frac{1}{2} \int_0^\pi f \sin \theta \, d\theta, \quad (8)$$

where θ is the angle between the electron momentum \mathbf{p} and the z axis.

The symmetric barrier is characterized by reflection and transmission coefficients, $R(\cos \theta)$ and $T(\cos \theta)$ respectively, identical for electrons incident from the left and from the right. These coefficients satisfy the relation

$$R(\cos \theta) + T(\cos \theta) = 1. \quad (9)$$

The reflection and transmission coefficients connect the distribution function at different sides of the barrier. Without a loss of generality, we can assume that the semiconductors at the left and right sides of the barrier occupy regions $z < 0$ and $z > 0$, respectively, in spite of the finite width of the barrier in reality. The momentum component parallel to the barrier is conserved both in reflection and transmission. This leads to the following boundary condition for the distribution function:

$$f(v_z)|_{z=+0} = R(\cos \theta) f(-v_z)|_{z=+0} + T(\cos \theta) f(v_z)|_{z=-0}, \quad (10)$$

$$v_z > 0,$$

$$f(v_z)|_{z=-0} = R(\cos \theta) f(-v_z)|_{z=-0} + T(\cos \theta) f(v_z)|_{z=+0},$$

$$v_z < 0.$$

Before presenting a mathematical solution to Eq. (7) we discuss qualitatively its structure. To calculate the resistance we solve the Boltzmann equation in linear approximation, i.e., assume that the distribution function has the form $f = f_0 + f_1$ where f_0 is the Fermi function and f_1 is a linear in electric field small correction describing a deviation from the equilibrium. Without a barrier the electric field is uniform across the whole structure and f_1 is an odd function of the electron momentum. This correction describes the current but does not change the energy distribution or the electron concentration. The barrier induces a nonuniformity of the electric field which, in a large scale, is equivalent to a discontinuity of the electric potential. More specifically, the potential distributions at both sides far from the barrier are linear in z but being extrapolated across the barrier these two linear functions are different by a constant value, $2\delta(e\phi)$. This potential drop is proportional to the electric field and equals zero in equilibrium.

We assume that an inelastic relaxation time is much larger than the elastic one and the Boltzmann equation [Eq. (7)] as well as the boundary conditions [Eqs. (10)] do not contain any energy relaxation mechanism. That is, Eqs. (7) and (10) describe an evolution of the electron distribution function along the z direction at a constant total energy. Electrons crossing the region of nonuniform field near the barrier change their kinetic energy to keep the total energy constant. At the other side of this region, where the electric field is uniform, the distribution function again is the equilibrium one plus the odd in the momentum correction. However, when we solve the Boltzmann equation we follow the distribution function along the z axis and express it in terms of the kinetic energy on one side of the barrier. After crossing the nonuniform field region, the distribution function at one side becomes expressed in terms of the kinetic energy on the other side. So far as the kinetic energies at different sides are different by $2\delta(e\phi)$ the new equilibrium distribution of the kinetic energy is different from that which electrons had before they crossed the barrier by $2\delta(e\phi)(df_0/dE_p)$. That is, for $|z| \rightarrow \infty$ we have $F(z) = F_\infty = \text{const}$, and

$$f_1 = -eF_\infty v_z \tau \frac{df_0}{dE} \pm \delta(e\phi) \frac{df_0}{dE}, \quad (11)$$

where E is the electron kinetic energy. The whole problem has a reflection symmetry with respect to the plane $z = 0$ and it is convenient to work with a symmetric solution. For this reason we choose a symmetric asymptotic solution taking the potential shift $\delta(e\phi)$ of different sign on opposite sides of the barrier. In other words, we express the distribution function in terms of the kinetic energy without the electric field; the latter shifts the energy on either side of the barrier so that far from the barrier the shift is $\pm\delta(e\phi)$. We remark that the asymptotic solution Eq. (11) exists only for $E > |\delta(e\phi)|$ because for a smaller kinetic energy there are no electron states on one side of the barrier. This remark must be taken into

account if one wishes to check that Eq. (11) gives the same electron concentrations on both sides of the barrier. Another remark is that Eq. (11) is not a boundary condition for the Boltzmann equation; on the contrary,

Eq. (11) naturally follows from the solution.

Equation (7) can be solved with respect to f_1 on each side of the barrier separately. The solution that is finite as $|z| \rightarrow \infty$ is of the form

$$f_1 = \begin{cases} A_+ e^{-z/v_z\tau} - \int_0^z e^{-(z-z')/v_z\tau} \left[eF(z') \frac{df_0}{dE} - \frac{1}{v_z\tau} \bar{f}_1(z') \right] dz' , & v_z > 0, \\ \int_z^\infty e^{-(z-z')/v_z\tau} \left[eF(z') \frac{df_0}{dE} - \frac{1}{v_z\tau} \bar{f}_1(z') \right] dz' , & v_z < 0, \end{cases} \quad (12)$$

for $z > 0$, and

$$f_1 = \begin{cases} \int_z^{-\infty} e^{-(z-z')/v_z\tau} \left[eF(z') \frac{df_0}{dE} - \frac{1}{v_z\tau} \bar{f}_1(z') \right] dz' , & v_z > 0, \\ A_- e^{-z/v_z\tau} - \int_0^z e^{-(z-z')/v_z\tau} \left[eF(z') \frac{df_0}{dE} - \frac{1}{v_z\tau} \bar{f}_1(z') \right] dz' , & v_z < 0, \end{cases} \quad (13)$$

for $z < 0$. Functions $A_+(v_z)$ and $A_-(v_z)$ are determined from the boundary conditions, expressed by Eq. (10):

$$A_+ = R(\cos\theta) \int_0^\infty e^{-z/v_z\tau} \left[eF(z) \frac{df_0}{dE} + \frac{1}{v_z\tau} \bar{f}_1(z) \right] dz + T(\cos\theta) \int_0^{-\infty} e^{z/v_z\tau} \left[eF(z) \frac{df_0}{dE} - \frac{1}{v_z\tau} \bar{f}_1(z) \right] dz , \quad v_z > 0, \quad (14)$$

$$A_- = R(\cos\theta) \int_0^{-\infty} e^{-z/v_z\tau} \left[eF(z) \frac{df_0}{dE} + \frac{1}{v_z\tau} \bar{f}_1(z) \right] dz + T(\cos\theta) \int_0^\infty e^{z/v_z\tau} \left[eF(z) \frac{df_0}{dE} - \frac{1}{v_z\tau} \bar{f}_1(z) \right] dz , \quad v_z < 0. \quad (15)$$

Substituting Eqs. (12)–(15) into Eq. (8) leads to an integral equation for the averaged function $\bar{f}_1(z)$. This equation is simplified by the symmetry relations

$$f_1(-v_z, -z) = -f_1(v_z, z), \quad A_-(-v_z) = -A_+(v_z), \quad \bar{f}_1(-z) = -\bar{f}_1(z). \quad (16)$$

In the degenerate electron gas, the averaged distribution function is factored into a product of functions, one depending on the energy, the other on the coordinate: $f_1 = eF_\infty l[\chi(\xi) \pm \Delta](df_0/dE)$, where $\delta(e\phi) = eF_\infty l\Delta$. It is convenient to introduce a dimensionless deviation of the electric field from its asymptotic value, $F(z) = F_\infty[1 + \tilde{F}(\xi)]$. Here $\xi = z/l$ is the dimensionless distance from the barrier and $l = v\tau$ is the mean free path of electrons moving with the Fermi velocity v . For $\xi > 0$, the resultant integral equation is of the form

$$2\chi(\xi) = 2 \int_\xi^\infty r(\xi') d\xi' - 2\Delta t(\xi) + \int_0^\infty [r(\xi + \xi') - t(\xi + \xi') - \text{sgn}(\xi - \xi')\Phi(|\xi - \xi'|)] \tilde{F}(\xi') d\xi' - \int_0^\infty [\Phi'(|\xi - \xi'|) + r'(\xi + \xi') - t'(\xi + \xi')] \chi(\xi') d\xi'. \quad (17)$$

The kernel is expressed in terms of the reflection and transmission coefficients as follows:

$$\begin{aligned} r(\xi) &= \int_0^{\pi/2} R(\cos\theta) e^{-\xi/\cos\theta} \sin\theta d\theta, \\ t(\xi) &= \int_0^{\pi/2} T(\cos\theta) e^{-\xi/\cos\theta} \sin\theta d\theta, \\ \Phi(\xi) &= r(\xi) + t(\xi) = \int_0^{\pi/2} e^{-\xi/\cos\theta} \sin\theta d\theta. \end{aligned} \quad (18)$$

Deviation of the electric field from its asymptotic value is determined by the Poisson equation

$$\frac{d\tilde{F}}{d\xi} = -\frac{l^2}{r_D^2} \chi, \quad (19)$$

where $r_D = (\pi\hbar^2\kappa/4me^2k)^{1/2}$ is the screening length, κ is the dielectric constant, and k is the Fermi wave vector.

Equations (17) and (19) determine the electron distribution and the electric field near the barrier. The value of

Δ is also determined from the integral equation and the conditions that $\chi(\xi) \rightarrow 0$ and $\tilde{F}(\xi) \rightarrow 0$ for $\xi \rightarrow \infty$. The current density is determined from the electron distribution far from the barrier, $j = \sigma F_\infty$, where $\sigma = e^2 \tau n / m$ is the conductivity and n is the electron concentration in the bulk. The resistance of the structure with the barrier is determined by the potential difference between two points that are far from the barrier on opposite sides. Then, according to our definition, the barrier resistance per unit area is given by

$$\begin{aligned} \mathcal{R} &= \frac{1}{j} \lim_{L \rightarrow \infty} \left\{ \int_{-L}^L F(z) dz + \frac{\delta(e\phi)}{e} - 2LF_\infty \right\} \\ &= \frac{6\pi^2 \hbar}{e^2 k^2} \left\{ \int_0^\infty \tilde{F}(\xi) d\xi + \Delta \right\}. \end{aligned} \quad (20)$$

For simplicity we neglect the potential drop across the barrier. This is justified if it is much smaller than the potential drop at the mean free path. This condition means that the width of the barrier has to be much smaller than the electron mean free path outside the barrier. Typically the mean free path in heterostructure devices is a few hundred angstroms or longer. That is, Eq. (20) is justified for a barrier of a few tens of angstroms. For a wider barrier the term $[1 + \tilde{F}(0)]d/l$ has to be added in brackets on the right-hand side, where d is the width of the barrier.

Equations (17) and (19) cannot be solved analytically for an arbitrary form of the reflection coefficient. An analytic solution, however, can be obtained in the limits of either strong or weak reflection.

IV. STRONG REFLECTION

In the limit $\mathcal{R} = 1$ (impenetrable barrier), the distribution functions on either side correspond to equilibrium and the electric field is zero. Because of the lack of electron exchange across the barrier the potential discontinuity between electron distributions at different sides of the barrier can be arbitrary. For a finite but strong reflection, the deviation from equilibrium is small, i.e., both $\chi(\xi)$ and $\tilde{F}(\xi)$ are small. Products of these functions and t are small to second order. It is convenient to eliminate $r(\xi)$ in the kernels of the integrals in Eq. (17) with the help of Eq. (18) and extend Eq. (17) to negative values of ξ , using the continuation

$$\chi(-\xi) = \chi(\xi), \quad \tilde{F}(-\xi) = -\tilde{F}(\xi). \quad (21)$$

Neglecting terms of the second order, we then have

$$\begin{aligned} \chi(\xi) &= \int_{|\xi|}^\infty r(\xi') d\xi' - \Delta t(|\xi|) \\ &\quad - \frac{1}{2} \int_{-\infty}^\infty \text{sgn}(\xi - \xi') \Phi(|\xi - \xi'|) \tilde{F}(\xi') d\xi' \\ &\quad - \frac{1}{2} \int_{-\infty}^\infty \Phi'(|\xi - \xi'|) \chi(\xi') d\xi'. \end{aligned} \quad (22)$$

Eliminating \tilde{F} with the help of Eq. (19) and taking the

Fourier transform of Eq. (22), we find

$$\begin{aligned} &\left(1 - \frac{\arctan q}{q}\right) \left(1 + \frac{l^2}{r_D^2 q^2}\right) \chi_q \\ &= 2 \int_0^1 R(x) \frac{x^2 dx}{1 + q^2 x^2} - 2\Delta \int_0^1 T(x) \frac{x dx}{1 + q^2 x^2}, \end{aligned} \quad (23)$$

where

$$\chi_q = \int \chi(\xi) e^{iq\xi} d\xi. \quad (24)$$

The inverse transformation gives

$$\begin{aligned} \tilde{F}(\xi) &= -\frac{l^2}{\pi r_D^2} \int_0^\infty \chi_q \frac{\sin q\xi}{q} dq \\ &= -\frac{l^2}{\pi r_D^2} \text{sgn}(\xi) \int_0^\infty \chi_{k/\xi} \frac{\sin k}{k} dk. \end{aligned} \quad (25)$$

$\tilde{F}(\xi)$ goes to zero at infinity only if $\chi_q = 0$ for $q = 0$. This means that the right-hand side of Eq. (23) must vanish at $q = 0$. This condition determines the value of Δ ,

$$\Delta = \left(\int_0^1 T(x)x dx \right)^{-1} \left[\frac{1}{3} - \int_0^1 T(x)x^2 dx \right]. \quad (26)$$

To first approximation, Eq. (23), then gives

$$\begin{aligned} \chi_q &\approx \frac{2}{1 - \frac{\arctan q}{q}} \frac{q^2}{q^2 + \frac{l^2}{r_D^2}} \\ &\quad \times \left[\frac{1}{q^2} \left(1 - \frac{\arctan q}{q}\right) \right. \\ &\quad \left. - \frac{1}{3} \left(\int_0^1 T(x)x dx \right)^{-1} \left(\int_0^1 T(x) \frac{x dx}{1 + q^2 x^2} \right) \right]. \end{aligned} \quad (27)$$

The integral in Eq. (20) is calculated with the help of Eq. (25) with the result

$$\begin{aligned} \mathcal{R} &= \frac{6\pi^2 \hbar}{e^2 k^2} \left\{ \left(\int_0^1 T(x)x dx \right)^{-1} \left[\frac{1}{3} - \int_0^1 T(x)x^2 dx \right] \right. \\ &\quad \left. - \frac{l^2}{r_D^2} \int_0^\infty \chi_q \frac{dq}{q^2} \right\}. \end{aligned} \quad (28)$$

The lowest-order approximation to Eq. (28) can be obtained by neglecting deviations from equilibrium.¹ In this case the current density across the barrier is

$$j = e\delta(e\phi) \int_{\cos\theta > 0} v_z T(\cos\theta) \frac{df_0}{dE} \frac{2d^3\mathbf{p}}{(2\pi\hbar)^3}, \quad (29)$$

which gives

$$\mathcal{R} = \frac{2\pi^2 \hbar}{e^2 k^2} \left(\int_0^1 T(x)x dx \right)^{-1}. \quad (30)$$

V. WEAK REFLECTION

In the case of zero reflection, Eq. (17) becomes homogeneous and χ , Δ , and \tilde{F} all vanish. For a finite but small reflection, the quantities χ , Δ , and \tilde{F} are small and products of these functions and r are small to second order. Neglecting these terms and extending Eqs. (17) and (19) to negative values of ξ through the continuation

$$\chi(-\xi) = -\chi(\xi), \quad \tilde{F}(-\xi) = \tilde{F}(\xi), \quad (31)$$

we bring Eqs. (17) into the form:

$$\begin{aligned} \chi(\xi) = & \operatorname{sgn}(\xi) \int_{|\xi|}^{\infty} r(\xi') d\xi' - \Delta \Phi(|\xi|) \operatorname{sgn}(\xi) \\ & - \frac{1}{2} \int_{-\infty}^{\infty} \operatorname{sgn}(\xi - \xi') \Phi(|\xi - \xi'|) \tilde{F}(\xi') d\xi' \\ & - \frac{1}{2} \int_{-\infty}^{\infty} \Phi'(|\xi - \xi'|) \chi(\xi') d\xi'. \end{aligned} \quad (32)$$

The Fourier transformation of this equation and Eq. (19) gives

$$\begin{aligned} & \left(1 - \frac{\arctan q}{q}\right) \left(1 + \frac{l^2}{r_D^2 q^2}\right) \chi_q \\ & = 2iq \left[\int_0^1 R(x) \frac{x^3 dx}{1 + q^2 x^2} - \frac{\Delta}{q^2} \left(1 - \frac{\arctan q}{q}\right) \right]. \end{aligned} \quad (33)$$

When q goes to zero, Eqs. (19) and (33) lead to

$$\int_{-\infty}^{\infty} \tilde{F}(\xi) d\xi = 6 \int_0^1 R(x) x^3 dx - 2\Delta, \quad (34)$$

where

$$\mathcal{R} = \frac{18\pi^2 \hbar}{e^2 k^2} \int_0^1 R(x) x^3 dx. \quad (35)$$

VI. SIMPLE MODEL

To estimate the effect of a deviation from equilibrium near the barrier, consider the model transmission coefficient

$$T(\cos \theta) = \frac{\cos^2 \theta}{a^2 + \cos^2 \theta}, \quad (36)$$

which is a good approximation for a high rectangular barrier.

If $a \gg 1$, then the reflection is strong and we have

$$\begin{aligned} \chi_q = & \frac{2}{q^2 + l^2/r_D^2} \left\{ 1 - \frac{2}{3} \left[1 - \frac{\ln(1 + q^2)}{q^2} \right]^{-1} \right. \\ & \left. \times \left(1 - \frac{\arctan q}{q} \right) \right\} \end{aligned} \quad (37)$$

and

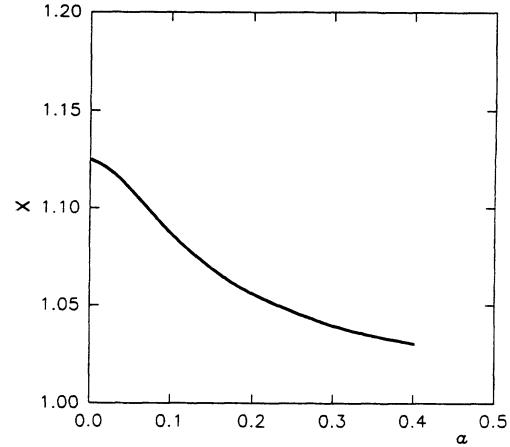


FIG. 2. Ratio X of the barrier resistance calculated exactly to that calculated with the Landauer formula, as a function of the barrier opaqueness parameter a .

$$\mathcal{R} = \frac{2\pi^2 \hbar}{e^2 k^2} \left(4a^2 + \frac{4}{15} - \frac{3l^2}{r_D^2} \int_0^{\infty} \chi_q \frac{dq}{q^2} \right). \quad (38)$$

In the opposite case, $a \ll 1$, we have

$$\mathcal{R} = \frac{2\pi^2 \hbar}{e^2 k^2} \frac{9a^2}{2} \left(1 - a^2 \ln \frac{1}{a^2} \right). \quad (39)$$

For the transmission coefficient of the form (36) the Landauer formula (1) gives

$$\mathcal{R} = \frac{2\pi^2 \hbar}{e^2 k^2} 4a^2. \quad (40)$$

Figure 2 shows a comparison between the exact expression and the usual Landauer formula, Eq. (40). For a very strong reflection only the first term can be kept in the parentheses in Eq. (38), and the latter reduces to Eq. (40). For a weak reflection, Landauer's expression is off by a numerical factor. The discrepancy would be much stronger for a nondegenerate electron gas, where the dependence of the relaxation time on energy is important.

VII. CONCLUSION

We have suggested a method for the calculation of the interface resistance in heterostructures which is a modification of the Landauer approach. Due to the effect of the interface on the electron scattering in its vicinity, it is impossible to make use of the Landauer formula with reflection and transmission coefficients of the interface. The calculation is reduced to an integral equation. We solved this equation for a simple model and found an appreciable difference compared to the classical Landauer formula.¹

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