Electronic transport through a planar defect in the bulk

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The extra resistivity ρ_{extra} due to a planar perturbation in an otherwise homogeneous bulk medium is considered. The current density incident on the barrier and the density distribution in the bulk are calculated self-consistently as a solution of a classical diffusion problem. Numerical calculations show fluctuations of the density within a few bulk mean free paths in the vicinity of the barrier. They depend sensitively on the transmission and reflection coefficients. Using the Einstein equivalence, we obtain ρ_{extra} from the long-range density drop across the barrier. The occurrence of the density fluctuations generally prevents the derivation of a simple generalization of the one-dimensional Landauer formula. Instead, a more involved expression for ρ_{extra} is found in a simplified model of discrete angles of carrier motion.

I. INTRODUCTION

Electronic transport in the presence of a localized perturbation of an otherwise homogeneous bulk system has attracted enhanced interest especially since Landauer's seminal 1957 paper.[1] The spatial variations of both electrical current and potential in the vicinity of the defect have been of special interest in the context of electromigration theory.[2,3] Unlike the now more popular viewpoint of two-terminal resistances,[4,5] where the voltage difference is measured between adjacent reservoirs feeding electrons into the device, the theory in its original formulation asked for the voltage difference inside the structure right across the obstacle, not involving the concept of reservoirs at all. The central idea in Ref. 1 was the formation of a current-induced dipole of carriers, called the residual resistivity dipole (RRD). This concept fell somewhat into oblivion when the two-terminal resistance became the focus of mesoscopic transport, particularly in ballistic structures. It is nevertheless a useful tool to investigate transport in systems that are intrinsically resistive such as bulk materials, quantum films, or resistive quantum wires. Here we will contribute to the original question and consider the extra resistance due to the RRD of a planar perturbation in a three-dimensional bulk system. Planar perturbations often serve as models for grain boundaries, stacking faults, or tunneling barriers.

A number of papers conceptually dealing with the RRD have appeared over the years. They can be roughly classified into three groups: (i) scatterers in one-dimensional or quasi-one-dimensional wires;[6–11] (ii) point defects in two- or three-dimensional bulk systems;[6,12–21] (iii) planar perturbations in three-dimensional bulk systems.[22–24]

Strictly one-dimensional systems seem to be well understood. Both classical[7,11] and quantum mechanical[6,10] approaches lead to the well-known $R/(1-R)$ expression for the extra resistance, where R is the reflection coefficient of the obstacle. It can be understood as the result of multiple attempts of reflected carriers to cross the barrier eventually. After an electron has been scattered by the obstacle, it also suffers scattering by the bulk and therefore has the chance to return to the obstacle where it contributes anew to the incident current. Summing up all these processes gives the above geometrical series. The problem of obstacles in multimode wires[8] is more involved. Recently, it has been tackled for the case of resistive quantum wires using a variational principle within a quasiclassical framework.[11] The derivation of a general expression for the resistance in resistive multimode wires turns out to be difficult.

The main issues of the work on the second topic are the formation of the RRD and the resulting electromigration field acting upon the impurity.[14,16] The calculations were restricted to effects of the first order in the scattering cross section. In Ref. 19 the Friedel oscillations in the vicinity of the scatterer were included. Recently, effects of higher order in the scattering cross section of the perturbation were addressed,[20,21] and the extra resistivity was found to depend on the transport cross section σ_T in a nonlinear fashion, $\rho_{\text{extra}} \sim \sigma_T/(1-\alpha\sigma_T)$. Here, too, the multiple scattering processes of carriers between obstacle and surrounding bulk lead to a geometrical series which is similar to the one-dimensional result. Since the carriers can bypass the perturbation, however, the nonlinear effect is far from being so pronounced as in a wire. The probability that carriers return to the obstacle is just expressed by the quantity $\alpha\sigma_T$ in the denominator of ρ_{extra}. Such a nonlinearity had been predicted long ago.[1,6]

The situation in the third group lies between the first two groups. Due to the extended bulk, the angles at which carriers can move form a continuum. On the other hand, due to the translational symmetry with respect to the barrier-bulk interface, it bears a resemblance to one-dimensional problems. To a certain extent, the system can be viewed as a wire with an infinite number of lateral modes. This has also been noted in recent work.[24] The similarity with one-dimensional problems implies that the carriers cannot bypass the barrier. One should therefore expect the resistivity to diverge like T^{-1}

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if the transmission coefficient T tends to zero for all angles of incidence. On the other hand, the continuum of angles suggests a certain averaging procedure for $R(\cos\theta)$ and $T(\cos\theta)$.

In Ref. 22 the Boltzmann theory is applied to a planar impurity layer sandwiched between reservoirs. Reference 23 shows the treatment of the transport problem through a barrier using a quantum mechanical superposition method[10] in the quasiclassical limit. The main result there is an analytical expression for the extra resistivity of the form $\langle R\rangle / \langle T\rangle$ containing simple angular averages of $R(\cos\theta)$ and $T(\cos\theta)$. It was obtained employing a diffusion picture, taking into account only the constant excess and deficit densities on both sides of the barrier. In Ref. 24, the Boltzmann distribution function was calculated, and it was found that, within some bulk mean free paths (MFP's) around the barrier, it depends sensitively on $R(\cos\theta)$ and $T(\cos\theta)$. The focus of Ref. 24 is that the angular distribution of the current density incident onto the barrier must be determined self-consistently including scattering processes both from the barrier and from the bulk scatterers. Taking this self-consistency approach seriously, it seems to be not possible to find a simple closed Landauer formula for the total range of R and T. In Ref. 24, analytical formulas for the extra resistivity could be derived for the limiting cases $R \ll 1$ and $T \ll 1$. The result for the second case was obtained under the assumption that the angle-dependent part of the current-induced distribution function around the barrier tends to zero in the limit $T \to 0$. While we confirm the result for the first case, we present arguments and numerical calculations which show that the said assumption for the second case is generally not correct. The situation $T = 0$, where the density distributions on both sides of the barrier are in equilibrium, cannot be connected by a perturbational method to the nonequilibrium case $0 < T \ll 1$ where a, current even though weak, flows. Both cases represent physically different situations. The same problem was encountered in the attempt to derive a general Landauer formula for obstacles in resistive multimode wires.[11]

In the present paper we treat the transport problem through a planar barrier using a classical kinetic equation and solving the arising diffusion problem self-consistently. We feel this method is particularly simple and transparent. The current is driven by a density gradient that takes a constant value far from the perturbation. Scattering of an incident current density from the barrier leads to a redistribution of carriers over all angles which deviates from the asymptotic distribution far from the barrier. Due to momentum relaxation in the bulk, a fraction of reflected particles returns to the barrier and forms anew an incident current. Therefore particle and current density can be obtained self-consistently from each other. The results obtained from the diffusion picture can be easily translated into the language of a force-driven current using the Einstein equivalence. The elastic bulk scattering is assumed to be isotropic and homogeneous. The condition that the Fermi wavelength is much smaller than the bulk mean free path justifies our classical model. A similar method has been used in recent works[11,20,21] where more details can be found.

As we did not succeed in deriving a complete solution of the resulting integrodifferential equations with a continuum of angles at which carriers can move, we solve them on an (arbitrarily fine) grid of discrete angles θ_n. Nevertheless, we are able to obtain all essential results from the discrete equations. Besides, we present numerical calculations of the density to support our conclusions.

In order to avoid misunderstanding it must be said that no direct comparison can be made between the results for a single barrier considered here and Landauer's considerations concerning an array of barriers and the characteristic velocity distribution between them.[1]

II. CLASSICAL KINETICS OF THE BULK

We adopt the model shown in Fig. 1 where the barrier is of zero thickness. According to our classical picture, the particle and current densities are

$$\varrho(\mathbf{r}) = \int_{4\pi} d\Omega\, \varrho(\mathbf{r},\Omega), \tag{1}$$

$$\mathbf{j}(\mathbf{r}) = \int_{4\pi} d\Omega\, \hat{\mathbf{e}}_\Omega\, j(\mathbf{r},\Omega), \tag{2}$$

where $\varrho(\mathbf{r},\Omega)$ and $j(\mathbf{r},\Omega)$ are the particle and current densities due to cariers moving in the direction of the unit vector $\hat{\mathbf{e}}_\Omega$. $\Omega = (\varphi,\theta)$ is the usual solid angle. $j(\mathbf{r},\Omega)$ and $\varrho(\mathbf{r},\Omega)$ are connected by the relation $j(\mathbf{r},\Omega) = v\varrho(\mathbf{r},\Omega)$. Due to the background scatterers, the carriers can change their direction of motion. This process is described by the

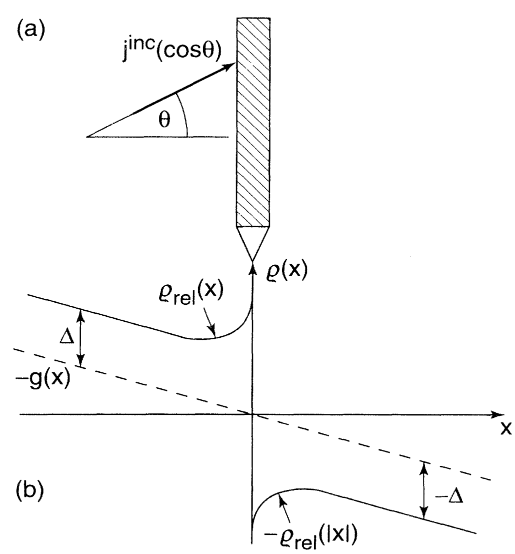

FIG. 1. (a) Schematic representation of the barrier with incident current density. (b) In the mathematical model, the thickness of the barrier is neglected (below). The symmetric density profile around the barrier consists of the asymptotic value $-gx$ (dashed), the constant part Δ of the excess density, and the exponentially decaying relaxation density $\varrho_{\rm rel}(x)$.

local kinetic equation

$$\mathbf{e}_\Omega \frac{\partial}{\partial \mathbf{r}} j(\mathbf{r},\Omega) = -\gamma \varrho(\mathbf{r},\Omega) + \frac{\gamma}{4\pi}\int_{4\pi} d\Omega' \varrho(\mathbf{r},\Omega'), \quad (3)$$

where γ is the bulk scattering rate. Let us define the quantities $\bar{\varrho}(\mathbf{r},\Omega) \equiv \varrho(\mathbf{r},\Omega) + \varrho(\mathbf{r},\Omega^*)$ and $\bar{j}(\mathbf{r},\Omega) \equiv v[\varrho(\mathbf{r},\Omega) - \varrho(\mathbf{r},\Omega^*)]$ where Ω^* is defined by $\mathbf{e}_{\Omega*} = -\mathbf{e}_\Omega$. With the kinetic equation for $\varrho(\mathbf{r},\Omega^*)$ and $j(\mathbf{r},\Omega^*)$, complementary to Eq. (3), and either adding or subtracting both equations, we find

$$\mathbf{e}_\Omega \frac{\partial}{\partial \mathbf{r}} \bar{\varrho}(\mathbf{r},\Omega) = -\frac{\gamma}{v^2}\bar{j}(\mathbf{r},\Omega) \quad (4)$$

and

$$\mathbf{e}_\Omega \frac{\partial}{\partial \mathbf{r}} \bar{j}(\mathbf{r},\Omega) = -\gamma\,\bar{\varrho}(\mathbf{r},\Omega) + \frac{\gamma}{4\pi}\int_0^{2\pi} d\varphi' \int_0^{\pi} d\theta' \sin\theta'\,\bar{\varrho}(\mathbf{r},\Omega'). \quad (5)$$

If the density gradient is constant, $\partial\varrho(\mathbf{r})/\partial\mathbf{r} = -g\hat{\mathbf{e}}_x$, we have $\bar{\varrho}(\mathbf{r},\Omega) = -gx/2\pi$, and the usual diffusion law follows from Eq. (4) with the diffusion constant $D = vl/3$ where $l = v/\gamma$ is the bulk MFP. Since the present problem is invariant with respect to translations parallel to the y-z plane, the differential operator $\hat{\mathbf{e}}_\Omega\,\partial/\partial\mathbf{r}$ is reduced to $\zeta\,\partial/\partial x$ where $\zeta = \cos\theta$. Moreover, due to the isotropy of the bulk scattering, the symmetry relation $\bar{\varrho}(x,\Omega) = \bar{\varrho}(x,\zeta) = \bar{\varrho}(x,-\zeta)$ holds. Then, combining Eqs. (4) and (5) gives

$$l^2\,\zeta^2\,\frac{\partial^2}{\partial x^2}\bar{\varrho}(x,\zeta) = \bar{\varrho}(x,\zeta) - \frac{1}{2}\int_{-1}^{1} d\zeta'\,\bar{\varrho}(x,\zeta'). \quad (6)$$

In the diffusion picture employed here, $\varrho(x)$ is determined up to an additive equilibrium density. However, we mean with $\varrho(x)$ the nonequilibrium part only.

We did not succeed in deriving a complete set of solutions of Eq. (6) in its continuous form. Therefore we solve it on a grid of discrete values ζ_n. If we divide the interval $[0 \le \zeta \le 1]$ into N equal parts, Eq. (6) reads

$$l^2\,\zeta_n^2\,\frac{\partial^2}{\partial x^2}\bar{\varrho}(x,\zeta_n) = \bar{\varrho}(x,\zeta_n) - \frac{1}{N}\sum_{m=1}^{N}\bar{\varrho}(x,\zeta_m). \quad (7)$$

Equation (7) resembles the second-order differential equation for the channel densities in a quantum wire considered in Ref. 11.

One solution of Eq. (7) is easily found if the left-hand side vanishes:

$$\bar{\varrho}_0(x,\zeta_n) = -\frac{g\,x}{2\pi N} + A^{r/l}. \quad (8)$$

The first term corresponds to the homogeneous diffusion process in the unperturbed bulk (cf. above), whereas the constant contribution accounts for the RRD, as we shall see later on. The superscript r/l indicates the side of the barrier. In the following, we will consider only the left-hand side, and therefore omit the superscript. To find a complete set of solutions of Eq. (7), we employ the ansatz

$$\bar{\varrho}(x,\zeta_n) = \hat{\varrho}_{\lambda n}\,e^{-\kappa_\lambda |x|}. \quad (9)$$

Inserting this into Eq. (7) leads to the linear eigenvalue problem

$$l^2\,\zeta_n^2\,\kappa_\lambda^2\hat{\varrho}_{\lambda n} = \hat{\varrho}_{\lambda n} - \frac{1}{N}\sum_{m=1}^{N}\hat{\varrho}_{\lambda m}, \quad (10)$$

the solutions of which can readily be written down, namely,

$$\hat{\varrho}_{\lambda n} = \frac{\beta_\lambda}{1-\kappa_\lambda^2 l^2 \zeta_n^2}. \quad (11)$$

β_λ is a normalization constant. From Eqs. (10) and (11) follows immediately $\sum_{m=1}^{N}\hat{\varrho}_{\lambda m} = N\beta_\lambda$. The solutions (9) describe the relaxation of a density distribution $\bar{\varrho}(x,\zeta_n)$ which deviates from the distribution (8) of the unperturbed bulk. Each eigenvalue κ_λ^2 corresponds to an eigenvector $\hat{\varrho}_{\lambda n}$ accounting for a narrow angular range around $\zeta_n = (\kappa_\lambda l)^{-1}$. $\hat{\varrho}_{\lambda n}$ has a maximum around that point. This is obvious from Eq. (11). It is also consistent with the notion that carriers moving at an angle θ should be relaxed after a distance $\kappa^{-1} \approx l\,\cos\theta$. Since it is the bulk background scattering that causes the relaxation, the upper limit to the relaxation lengths κ_λ^{-1} is of order l. The eigenvalue spectrum can be checked numerically. We find indeed that $\kappa_\lambda^{-1} \le l$.

We can formally write the constant part of the homogeneous solution (8) as $\hat{\varrho}_{0n}\exp(-\kappa_0|x|)$ where $\hat{\varrho}_{0n} = \beta_0$ and $\kappa_0 = 0$. From the symmetry of Eq. (7) follows then immediately the orthogonality relation

$$\sum_{n=1}^{N}\hat{\varrho}_{\lambda n}\,\zeta_n^2\,\hat{\varrho}_{\lambda' n} = \delta_{\lambda\lambda'}, \quad \lambda,\lambda' = 0,...,N-1, \quad (12)$$

where the normalization has been at once suitably fixed.

Any density distribution $\bar{\varrho}(x,\zeta_n)$ on either side of the barrier can be represented as a superposition

$$\bar{\varrho}(x,\zeta_n) = -\frac{gx}{2\pi N} + \sum_{\lambda=0}^{N-1} C_\lambda\,\hat{\varrho}_{\lambda n} e^{-\kappa_\lambda |x|}. \quad (13)$$

The total density is therefore

$$\varrho(x) = -gx + 2\pi\sum_{\lambda=0}^{N-1} C_\lambda\,N\,\beta_\lambda\,e^{-\kappa_\lambda |x|}. \quad (14)$$

We will call the sum in Eq. (14) for $x < 0$ the excess density and, accordingly, the deficit density for $x > 0$. The sum in Eq. (14) which excludes the term $\lambda = 0$ is called the relaxation density $\varrho_{\rm rel}(x)$ (see Fig. 1).

The coefficients C_λ must be determined so as to fulfill the boundary condition $\bar{\varrho}(0,\zeta_n) = \bar{\varrho}^B(\zeta_n)$ on the barrier interface. If $\bar{\varrho}(0,\zeta_n)$ matches the boundary condition, $\bar{\varrho}(x,\zeta_n)$ describes the correct density distribution in the corresponding half space. $\bar{\varrho}^B(\zeta)$ will be considered below. For the moment, we assume it to be given. The coefficients C_λ can then be obtained by using the orthonormality relation (12),

$$C_\lambda = \sum_{n=1}^{N} \hat{\varrho}_{\lambda n}\, \zeta_n^2\, \bar{\varrho}^B(\zeta_n). \tag{15}$$

From Eq. (14) we see that the coefficients C_λ with $\lambda \neq 0$ determine the density fluctuation within a few MFP's around the barrier, whereas C_0 corresponds to the long-ranged density change. $2\pi N\beta_0 C_0 \equiv \Delta$ can therefore be viewed as Landauer's RRD which determines the additional resistance due to a perturbation.

Let us now consider how the boundary condition $\bar{\varrho}^B(\zeta_n)$ on the barrier can be obtained from the current density incident on the barrier. The latter is assumed to be internally homogeneous and ideally smooth. The reflection and transmission coefficients, $R(\zeta_n)$ and $T(\zeta_n)$, obey then the relation

$$R(\zeta_n) = 1 - T(\zeta_n). \tag{16}$$

If the barrier were inhomogeneous[25] or rough,[26] the reflection and transmission coefficients would contain off-diagonal elements.

If a current density $j^{\rm inc}(\zeta_n)$ is incident on the barrier, the density at the left interface is

$$\bar{\varrho}^B(\zeta_n) = [1 + R(\zeta_n) - T(\zeta_n)]\, \frac{j^{\rm inc}(\zeta_n)}{v}. \tag{17}$$

The minus sign in front of $T(\zeta_n)$ is due to the antisymmetry of the nonequilibrium density $\varrho(x)$ with respect to x, i.e., $\varrho(x) = -\varrho(-x)$. Currents from the right half space must be counted negative. $j^{\rm inc}(\zeta_n)$ in turn can be calculated from the density $\varrho(x)$ using the kinetic equation (3) in its integral, yet discretized form, i.e.,

$$j^{\rm inc}(\zeta_n) = \frac{v}{4\pi N l} \int_0^{-\infty} \frac{dx}{\zeta_n}\, e^{-|x|/l\zeta_n}\, \varrho(x). \tag{18}$$

We can replace $\varrho(x)$ in Eq. (18) by the superposition (14). With Eqs. (17) and (16) we obtain for the density distribution $\bar{\varrho}^B(\zeta_n)$ on the barrier interface

$$\begin{aligned}\bar{\varrho}^B(\zeta_n) &= \sum_{\lambda=0}^{N-1} C_\lambda \hat{\varrho}_{\lambda n} \\ &= R(\zeta_n) \left[-\frac{g\, l\, \zeta_n}{2\pi N} + \sum_{\lambda=0}^{N-1} C_\lambda\, \beta_\lambda\, \frac{1}{1 + \kappa_\lambda\, l\, \zeta_n} \right],\end{aligned} \tag{19}$$

where the integration over x in Eq. (18) has been carried out. The right-hand side is just the expansion of $\bar{\varrho}^B(\zeta_n)$ into the eigenvectors $\hat{\varrho}_{\lambda n}$. It is hence possible to determine the coefficients C_λ and thus the density self-consistently. Note that the inhomogeneity in Eq. (19), proportional to the asymptotic density gradient g, fixes the total current through the barrier. If we apply the projection procedure (15), we arrive at the linear equation system

$$\sum_{\lambda=0}^{N-1} A_{\lambda\lambda'}\, C_{\lambda'} = G_\lambda, \tag{20}$$

where

$$A_{\lambda\lambda'} = \delta_{\lambda\lambda'} - \beta_{\lambda'} \sum_{n=1}^{N} \frac{\hat{\varrho}_{\lambda n}\, \zeta_n^2}{1 + \kappa_{\lambda'} l \zeta_n}\, R(\zeta_n) \tag{21}$$

and

$$G_\lambda = \frac{g\, l}{2\pi N} \sum_{n=1}^{N} \hat{\varrho}_{\lambda n}\, \zeta_n^3\, R(\zeta_n). \tag{22}$$

Using Cramer's rule,[27] we can express the solution C_λ as the ratio of two determinants, namely,

$$C_\lambda = \frac{\det(A_{\lambda\to G})}{\det(A)} = \frac{\displaystyle\sum_{\lambda'=0}^{N-1} a_{\lambda\lambda'} G_{\lambda'}}{\displaystyle\sum_{\lambda'=0}^{N-1} a_{\lambda\lambda'} A_{\lambda\lambda'}}. \tag{23}$$

$A_{\lambda\to G}$ denotes the matrix A where the λth column has been replaced by the vector G_λ. The $a_{\lambda\lambda'}$ are the corresponding cofactors.[27] For the resistance (see Sec. III), we are particularly interested in the coefficient C_0 of the long-range density change or, respectively, in the density dipole Δ. With relations (12) and (16) we find for the corresponding column $\lambda' = 0$ of $A_{\lambda\lambda'}$

$$A_{\lambda 0} = \sum_{n=1}^{N} \hat{\varrho}_{\lambda n}\, \zeta^2\, T(\zeta_n). \tag{24}$$

C_0 is then

$$C_0 = \frac{g\, l}{2\pi N \beta_0} \frac{\displaystyle\sum_{\lambda=0}^{N-1} a_{\lambda 0} \sum_{n=1}^{N} \hat{\varrho}_{\lambda n}\, \zeta_n^3\, R(\zeta_n)}{\displaystyle\sum_{\lambda=0}^{N-1} a_{\lambda 0} \sum_{n=1}^{N} \hat{\varrho}_{\lambda n}\, \zeta_n^2\, T(\zeta_n)}. \tag{25}$$

Note that the cofactors $a_{\lambda 0}$ also depend on $R(\zeta_n)$ and $T(\zeta_n)$. Equation (25) expresses therefore no simple averaging of R and T but a considerably more complex procedure. It can be simplified only in certain limiting cases; see Sec. IV. Generally, the total density variation is established after many scattering cycles from the barrier back into the bulk. In each cycle, all directions of motion are mutually coupled according to the kinetic equation (3). The complex interplay of all scattering cycles prevents a simple averaging scheme for $R(\zeta)$ and $T(\zeta)$ as proposed, for example, in Ref. 23. We also point out that the dipole moment $\Delta = 2\pi N\beta_0 C_0$ does not depend on N if the resolution is fine enough to sample all variations of $R(\zeta_n)$ and $T(\zeta_n)$. This has been checked numerically.

III. EXTRA RESISTIVITY

Here we show briefly how the results of the diffusion picture considered throughout this paper can be translated into the conventional picture of a force-driven electrical current. To this purpose, we employ the quantity $u(x) = \varrho(x)/n(E_F)$ rather than the density itself. $n(E_F) = m^2 v_F/2\pi^2\hbar^3$ is the local density of states. We restrict ourselves to the zero temperature limit. Then all quantities must be taken at the Fermi surface. The difference $\delta u(-x) - \delta u(x)$, introduced by the barrier, leads to an additional drop $e\Phi$ of the electrostatic potential which is established within some microscopic screening lengths across the barrier. For a large distance L from the interfaces, i.e., $L \gg l$, the difference $\delta u(-L) - \delta u(L)$ is constant,

$$\delta u(-L) - \delta u(L) = \frac{2\Delta}{n(E_F)}. \tag{26}$$

In this region it is sensible to define the extra resistivity ρ_{extra} as ratio of $[\delta u(-\infty) - \delta u(+\infty)]$ to the electronic currrent density $|\mathbf{j}|$ driven through the system. $|\mathbf{j}|$ is given by the diffusion law as $|\mathbf{j}| = g\, l\, v_F\, e/3$. Thus we get for the extra resistance

$$\rho_{\mathrm{extra}} = \frac{3h^3}{2\pi e^2 v_F^2 m^2}\frac{\Delta}{gl}. \tag{27}$$

We note that the *total* carrier density in a real transport situation is constant (over distances large compared to the screening length). If the screening length is much shorter than the bulk MFP (as is mostly the case in metals), the band bottom mirrors the density fluctuations found in our diffusion picture.

IV. RESULTS AND LIMITING CASES

Consider first the limit of a weakly scattering barrier ($R \ll 1$). In this case the cofactors of the first column are $a_{\lambda 0} = \delta_{\lambda 0} + O(R)$, where R means the typical order of $R(\zeta)$. We insert this into Eq. (25) and replace the summations over n with integrations over ζ. Then we get

$$\rho_{\mathrm{extra}} = \frac{9h^3}{2\pi e^2 v_F^2 m^2}\int_0^1 d\zeta\, \zeta^3\, R(\zeta). \tag{28}$$

This result has been obtained also by other authors using different methods.[23,24] The situation here is relatively simple since the current density incident on the barrier can be replaced by the unperturbed bulk current density. A perturbation approach is possible, and higher-order effects can be neglected. The relaxation density can be obtained directly from Eq. (20) and of order $g\, l\, O(R)$.

The situation changes drastically if we consider the opposite limit of a strong barrier ($T \ll 1$). Here a perturbation expansion definitely fails. Figure 2 shows the normalized excess density $[\varrho(x) + g\, x]/gl$ where the coefficients C_λ in Eq. (14) have been calculated numerically from Eq. (23). We use the same model transmission coefficient as in Ref. 24, namely,

$$T(\zeta) = \frac{\zeta^2}{\alpha^2 + \zeta^2} \tag{29}$$

with $\alpha^2 = 10^3$. The relaxation density ϱ_{rel} is roughly of

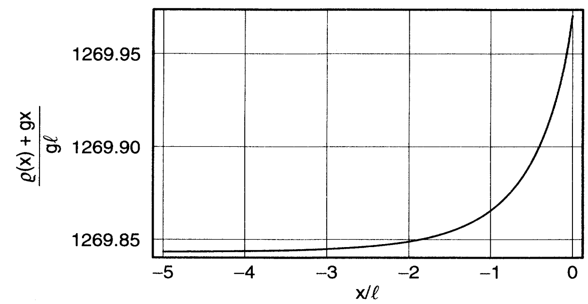

FIG. 2. Normalized excess density on the left-hand side of the model barrier described by Eq. (29). While Δ is of order $g\, l\, T^{-1}$, the relaxation density is of order $g\, l$. The resolution is $N = 10$.

order gl within a few mean free paths around the barrier before it exponentially vanishes. The dipole moment Δ, on the other hand, is of order $g\, l\, \alpha^{-2}$.

Using Eq. (23), we can qualitatively understand the orders of magnitude of ϱ_{rel} and Δ. One easily convinces oneself that the cofactors $a_{\lambda 0}$ become independent of $T(\zeta_n)$ in the limit $T \to 0$. The dependence of C_0 on $T(\zeta_n)$ is then only determined by the terms $\sum_n \hat{\varrho}_{\lambda n}\, \zeta_n^2\, T(\zeta_n)$ in the denominator in Eq. (25). We find that C_0 diverges like T^{-1} if T tends to zero. This is obvious from Fig. 2. On the other hand, we find after a little calculation from Eqs. (21), (22), and (23) that $C_\lambda \sim gl/N\beta_\lambda$ for all $\lambda \neq 0$. Therefore the relaxation density is generally of the same order as gl. This is also visible in Fig 2. Therefore the relaxation density must be taken into account when we determine the incident current density, even in the limit of weak transmission through the barrier.

The aforesaid, however, means that we do not recover the simple resistance formula derived in Ref. 24 (and, earlier, in Ref. 23) for the limit $T \ll 1$. Instead, the determinants in Eq. (25) must be calculated to obtain the correct extra resistance. ρ_{extra} is proportional to T^{-1}, of course, but its actual value depends on $T(\zeta)$ and $R(\zeta)$ in a more complex fashion.

The reason for this discrepancy is, in our opinion, the assumption $\varrho_{\mathrm{rel}} \sim T$ made in Ref. 24 [where the quantity $\chi(\xi)$ corresponds to the relaxation density $\varrho_{\mathrm{rel}}(x)$]. We present a simple calculation in order to make this point more transparent. Going back to the the continuous kinetic equation in integral form, we write down the density distribution $\bar{\varrho}^B(\zeta)$ at the left-hand side interface of the barrier,

$$\begin{aligned}\bar{\varrho}^B(\zeta) &= [1 - T(\zeta)]\left[\frac{g\, l\, \zeta + \Delta}{2\pi} + \frac{j_{\mathrm{rel}}^{\mathrm{inc}}(\zeta)}{v}\right] \\ &= \frac{\Delta}{2\pi} + \bar{\varrho}_{\mathrm{rel}}(0, \zeta)\end{aligned} \tag{30}$$

or, rearranging the terms,

$$\begin{aligned}T(\zeta)\Delta - g\, l\, R(\zeta)\, \zeta = 2\pi\{&[1 - T(\zeta)]\, v^{-1} j_{\mathrm{rel}}^{\mathrm{inc}}(\zeta) \\ &- \varrho_{\mathrm{rel}}(0, \zeta)\} \sim \varrho_{\mathrm{rel}}.\end{aligned} \tag{31}$$

$j_{\mathrm{rel}}^{\mathrm{inc}}(\zeta)$ is the contribution of the relaxation density to the incident current density and is proportional to ϱ_{rel}. From

Eq. (31) it is clear that the relaxation density must be generally of order $g\,l$. It is also clear that no perturbation approach can be used in order to connect the two cases $T = 0$ (where $g = 0$) and $0 < T \ll 1$ (where $g \neq 0$). The asymptotic current which forms the inhomogeneity in the self-consistency integral equation (Ref. 24) or equation system [Eq. (19)] jumps from zero to a finite value.

We want to emphasize that the disagreement between the results presented in Refs. 23 and 24 and our results in the $T \ll 1$ limit only results in a factor of order 1. This can be seen qualitatively from Eq. (31), too. Whether we include $\varrho_{\rm rel}$ or not in the calculation of Δ does not change the order of magnitude of the extra resistance. This makes it hard to devise experiments that could prove the correctness of our result. Such measurements would require that the parameters of a planar barrier be exactly known. This, however, is difficult to achieve in practice.

In the special case $T(\zeta_n) = T_0\zeta_n$, $T_0 \ll 1$, Eq. (25) becomes particularly simple and we find

$$\rho_{\rm extra} = \frac{3h^3}{2\pi e^2 v_F^2 m^2\, T_0}. \tag{32}$$

Equation (32) exactly reproduces the result found by Laikhtman and Luryi.[24] From Eqs. (30) and (31), it is also easy to see why the relaxation density vanishes if $T(\zeta) \sim \zeta$. Then the barrier transmission exactly fits the angular distribution of the incident current density, $g\,l\,\zeta + \Delta$ (up to small corrections $\sim T_0^2$). No relaxation is needed to redistribute reflected or transmitted carriers.

Finally we want to discuss the density profile around a barrier with a transmission window in a narrow angular range. We choose a model transmission coefficient of the form $T(\zeta_n) = T_0$ if $\zeta_n = \zeta_0$, and zero otherwise. Even though such a model might seem too academic, it provides some interesting insights. Figure 3 shows the excess density due to the barrier for four different transmission windows. From curve (a) to curve (d), the transmission angle increases. We notice two significant features. First, the density dipole moment Δ and thus the extra resistance increase with the angle of the transmission window. [Note the different offsets of curves (a)–(d) for better representation.] This is appealing since the contribution of particles moving at an angle θ to the total current decreases as $\cos\theta$. The second, more interesting observation is that the profile of the excess density changes with ζ_0. For perpendicular transmission, as in curve (a), the relaxation density increases towards the barrier. At oblique transmission, as in curve (d), the density drops at the interface. Finally, for a transmission window around $\zeta_0 \approx \cos(\pi/4)$, the relaxation density shows a nonmonotonic behavior with a local minimum. This is shown in curves (b) and (c).

Now we want to give a simple qualitative explanation of the density in Fig. 3 curves (b) and (c). The discussion of the other cases is straightforward. Consider Fig. 4 where $\bar\varrho(x,\zeta_n)$ has been depicted in a simplified model of only three directions $\theta_1 < \theta_2 < \theta_3$. The barrier has a transmission window at θ_2. Figure 4(a) shows $\bar\varrho(0,\zeta_n)$, i.e., at the left interface. Since carriers moving towards the barrier at an angle θ_2 can easily leave the left half space without being compensated by carriers from the right half space, $\bar\varrho(0,\zeta_2)$ is lower than the average $\langle\bar\varrho(0,\zeta_n)\rangle$ over all angles. In Sec. II we have seen that carriers moving at an angle θ are relaxed after a distance $l\cos\theta$ [see the remarks after Eq. (11)]. Thus after a distance $l\zeta_3$, as shown in Fig. 4(b), we have $\bar\varrho(l\zeta_3,\zeta_3) \approx \langle\bar\varrho(l\zeta_3,\zeta_n)\rangle$. The average density, however, is

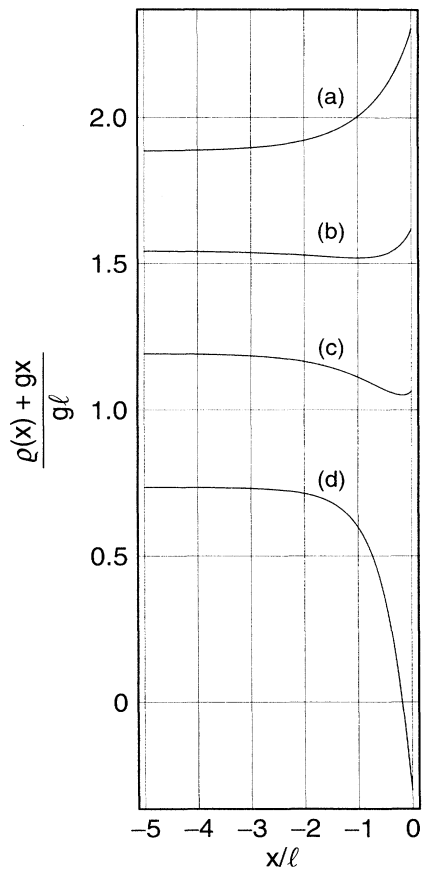

FIG. 3. Excess density on the left-hand side of the barrier for different transmission windows. Appropriate offsets ensure that all curves can be represented in a single diagram. At θ_0, $T_0 = 0.5$, and is zero otherwise. Curve (a) $\theta_0 = 0°$, offset 4.5; curve (b) $\theta_0 = 38°$, offset 7.0; curve (c) $\theta_0 = 46°$, offset 9.0; curve (d) $\theta_0 = 68°$, offset 19.5. The resolution is in all cases $N = 10$.

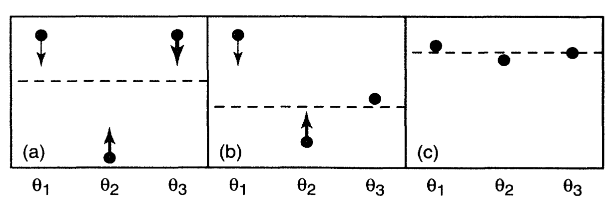

FIG. 4. Density distribution for three distances x from the barrier in a simple three-angle model. (a) $x_1 = 0$; (b) $x_2 \approx l\zeta_3$; (c) $x_3 \approx l\zeta_2$. The dashed line denotes the density averaged over n, i.e., $\langle\bar\varrho(x_i,\zeta_n)\rangle_n$. Thicker arrows indicate faster relaxation between two steps x_i and x_{i+1} than thinner ones. See text for further explanations.

now lower than it was at $x = 0$. At a distance $l\zeta_2$ then, the relaxation of carriers moving at ζ_2 has again led to a rise of the average density. Thus the joint endeavor of carriers at minimizing deviations of their partial density from a common average, on the one hand, and the different lengths needed to reach this relaxation, on the other hand, lead to the characteristic density profiles shown in Fig. 3.

V. CONCLUSIONS

Our investigation of the carrier density around a planar perturbation in the bulk has revealed fluctuations within a few MFP's. These fluctuations can be calculated self-consistently and are sensitive to the angular dependence of the barrier transmission and reflection coefficients. Numerical calculations show that the density near the barrier can exhibit concave, convex, or even a nonmonotonic shape, depending on $R(\zeta)$ and $T(\zeta)$. In the limit of a weak barrier, we have confirmed the result for the extra resistivity ρ_{extra} found in Refs. 23 and 24. However, the derivation of a generalized Landauer formula, containing simple angular averages of $R(\zeta)$ and $T(\zeta)$, seems generally not possible. Within our discrete angle model, we have instead derived an expression for the extra resistivity of the barrier that requires the calculation of determinants containing $R(\zeta_n)$ and $T(\zeta_n)$ [Eq. (25)]. It can be used for practical calculations of ρ_{extra}. Whether the discrete formalism developed here can be translated into a continuous form remains a mathematical task for future investigations.

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