

Obstacles in three-dimensional bulk systems: The residual-resistivity-dipole problem

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The problem of the residual resistivity dipole formulated by Landauer in 1957 is reconsidered for a spherically symmetric obstacle which is small compared to the bulk mean free path but otherwise arbitrary. A classical formalism is developed which rests on a local kinetic equation. The current density incident on the obstacle is the central quantity that allows us to calculate all relevant quantities. It is obtained self-consistently. The current-induced density dipole (and thus the additional resistance) is found to depend in a nonlinear fashion on the scattering cross section of the obstacle. This nonlinearity is similar to the well-known expression $R/(1 - R)$ for the one-dimensional case but is far from being so pronounced since in higher dimensionals the carriers can circumvent the obstacle.

I. INTRODUCTION

In his seminal 1957 paper,¹ Landauer formulated the question of how the resistance of a system is changed by an additional obstacle. The basic idea was that of the so-called residual resistivity dipole (RRD), which means that carriers are piled up on the forefront of the obstacle and that there is a density deficit behind. This gives rise to a long-range density dipole and thus to an additional resistivity, as a density difference is connected with a difference of chemical potentials via the Einstein equivalence.

For one-dimensional (1D) systems, the problem can be solved analytically for ballistic as well as for diffusive transport in the surroundings of the obstacle.¹⁻³ In both cases, the additional resistance has been found to be proportional to $|r|^2/(1 - |r|^2)$, where $|r|^2$ is the reflection coefficient of the obstacle. One possible explanation of the enhancement factor $(1 - |r|^2)^{-1}$ uses the idea of multiple scattering cycles between the obstacle and its surroundings, which can be described by a geometrical series. Particles reflected by the obstacle can be scattered by the surroundings and they thus have the chance to return to the obstacle where the next cycle begins. In order to avoid any potential misunderstanding, we emphasize that in the present context multiple scattering means scattering of intensities like current densities, in contrast to scattering of amplitudes in a wave theory. Using a wave superposition method in the quasiclassical limit, i.e., if the electron wavelength λ is much smaller than the bulk mean free path (MFP) l , Lenk³ determined the carrier density in a strictly one-dimensional system by a quantum-mechanical self-consistency scheme. As the carriers cannot bypass the obstacle, the limit of an opaque obstacle leads to infinite resistance. In the opposite limit of ideal transmission through the obstacle, the additional resistance vanishes. A situation similar to the strict one-dimensional case is that of a planar defect, of-

ten used as a model for grain boundaries. In Ref. 4 such a planar defect was considered, assuming a constant excess or deficit carrier density on either side of the barrier. Most recently, Laikhtman and Luryi⁵ pointed out that these current-induced densities are not constant but vary within few mean free paths in the vicinity of the barrier. In both papers, the extra resistance due to the barrier has been found to depend on the reflection coefficient in a way $\langle |r(\theta)|^2 \rangle / [1 - \langle |r(\theta)|^2 \rangle]$, where $\langle \rangle$ means angular averaging over a half sphere with appropriate weights following from the corresponding assumptions on the bulk scattering mechanisms (in Ref. 5, such closed expressions have been obtained only for the limits of small and large $|r|^2$). These results, too, can be interpreted by the multiple attempts of reflected carriers to cross the barrier.

Because the idea of the said multiple scattering cycles is not restricted to the one-dimensional case, it is tempting to develop a formalism which applies also to higher dimensionality. This is the aim of the present paper. It will be shown that in the 3D bulk, too, the interaction of an obstacle with its surroundings leads to an enhancement factor similar to that of the 1D case. This is physically appealing, as the current incident on the obstacle comprises, on one side, an additional contribution caused by the piled-up density, whereas on the other side the incident current is diminished by the density deficit. Thus, it is clear that the resistivity will depend on the scattering cross section σ in a nonlinear manner. This nonlinearity, however, is far from being as pronounced as in the 1D case, because the carriers can bypass the obstacle. Landauer predicted a resistivity which is proportional to an effective scattering cross section,

$$\tilde{\sigma} = \sigma / (1 - \alpha\sigma), \quad (1)$$

where $\alpha\sigma$ is a measure for the importance of the multiple scattering cycles.^{1,6} Below we will derive such a formula. We believe this is the first time that an explicit

and analytical expression for the RRD (and, thus, for the additional resistivity) of an arbitrarily strong obstacle is found. Sorbello and Chu^{7,8} considered the RRD and the electromigration force on an obstacle in a quasi-two-dimensional film. Their calculations were restricted to the first order with respect to the incident current density. A recent paper by Zwerger *et al.*⁹ presents an interesting quantum-mechanical approach to the RRD problem including the Friedel oscillations around the impurity. However, higher order processes were not yet incorporated in Ref. 9. Here, we will show how to include them in a closed and simple scheme.

Even though the self-consistent wave superposition method in its quasiclassical limit³ was successful in the one-dimensional case¹⁰ and in three-dimensional structures with planar defects,⁴ it seems difficult to handle the mathematical problems arising with higher dimensionality. Therefore, we tackle the problem anew by using a classical approach. This means here that the bulk is described by classical kinetics. A similar approach has been used recently¹¹ in order to handle transport through resistive multichannel quantum wires. More details on the main assumptions and the underlying physical concept can be found there. Here, we give only a rough survey.

(i) The system is filled with a uniform, weakly and isotropically scattering background, which gives rise to a finite MFP l and, thus, to a bulk resistivity. The de Broglie wavelength of the carriers is much smaller than the MFP. This justifies to treat the bulk classically.¹² In Refs. 3, 4, and 10, configurationally averaged elastic point scatterers are employed to model the bulk within a quantum-mechanical theory in its quasiclassical limit. Similarly, elastic bulk scattering is assumed to be dominant in Ref. 5 in a Boltzmann approach.

(ii) The diffusion case rather than the force case is considered. The transformation of the results to the usual force case is done by the Einstein equivalence. In a diffusion problem, it is always possible to add an equilibrium density without any change of the results.

(iii) We restrict our theory to the limit of zero temperature. In this case, only particles on the Fermi surface contribute to the transport.

(iv) In our classical model, all interference effects are neglected which would be important in a quantum-mechanical treatment,⁹ even after a configurational averaging of the background scatterers.^{3,4,10} This seems to be well justified since we are only interested in long-range density variations (i.e., if $r \gg l$). In Ref. 3, it was shown using a rigid theory that the oscillatory density fluctuations occurring around an obstacle in a quantum-mechanical description are of no importance for the *long-range* behavior of the density.

The basic ingredient of the present paper is a classical local kinetic equation from which all other equations can be obtained. Under the assumption that the obstacle is much smaller than the bulk MFP, we can separately solve a near-field and a far-field problem, similar to Refs. 7 and 8. Combining both procedures allows to construct a self-consistency scheme, for the incident current density, which will be solved analytically. Then, we calculate the RRD and finally the resistance. Since it makes no sense

to attribute a resistivity to a single scatterer in the infinite bulk, we consider a random distribution of identical obstacles over the entire space.

II. KINETICS OF THE BULK

The particle density $\varrho(\mathbf{r})$ and the current density $\mathbf{j}(\mathbf{r})$ are obtained by integrating over the solid angle Ω at the point \mathbf{r} :

$$\varrho(\mathbf{r}) = \int d\Omega \varrho(\mathbf{r}, \Omega), \quad (2)$$

$$\mathbf{j}(\mathbf{r}) = \int d\Omega \hat{\mathbf{e}}_{\Omega} j(\mathbf{r}, \Omega), \quad (3)$$

where $\hat{\mathbf{e}}_{\Omega}$ is the unit vector of the solid angle Ω . $\varrho(\mathbf{r}, \Omega)$ and $\mathbf{j}(\mathbf{r}, \Omega)$ are the particle and current densities at point \mathbf{r} , due to particles moving in the direction $\hat{\mathbf{e}}_{\Omega}$. Here and throughout the paper, the integration over the solid angle Ω is meant to be over the full sphere. Currents and densities are connected by the simple relation $j(\mathbf{r}, \Omega) = v \varrho(\mathbf{r}, \Omega)$, with v as the particle velocity. Note that this decomposition implies the neglect of all quantum-mechanical interferences.

Consider first the kinetics of the unperturbed bulk, i.e., without obstacle. The bulk scattering mechanism allows for transitions between different directions of motion. These scattering processes are assumed to be isotropic. In order to describe them, we introduce the transition rate γ . Then we can write down the simple local kinetic equation,

$$\hat{\mathbf{e}}_{\Omega} \frac{\partial}{\partial \mathbf{r}} j(\mathbf{r}, \Omega) = -\gamma \varrho(\mathbf{r}, \Omega) + \frac{\gamma}{4\pi} \varrho(\mathbf{r}). \quad (4)$$

In its integral form, the kinetic equation reads

$$j(\mathbf{r}, \Omega) = \frac{\gamma}{4\pi} \int_0^{\infty} d\tilde{r} e^{-\frac{\tilde{r}\gamma}{v}} \varrho(\mathbf{r} - \tilde{r} \hat{\mathbf{e}}_{\Omega}), \quad (5)$$

and we can express the current density as

$$\mathbf{j}(\mathbf{r}) = -\frac{v}{4\pi} \int d\Omega \int_0^{\infty} d\tilde{r} e^{-\frac{\tilde{r}\gamma}{v}} \hat{\mathbf{e}}_{\Omega} \left(\hat{\mathbf{e}}_{\Omega} \frac{\partial}{\partial \mathbf{r}} \right) \varrho(\mathbf{r} - \tilde{r} \hat{\mathbf{e}}_{\Omega}), \quad (6)$$

where the density gradient comes from a partial integration with respect to \tilde{r} . Here, we see that the density gradient determines the current density in a generally nonlocal manner. Only in the case that the density gradient is constant within a range of order v/γ around \mathbf{r} , the diffusion law holds in its usual simple form with the bulk diffusivity $D = vl/3$, where $l = v/\gamma$.

For $\varrho(\mathbf{r})$, we can derive a second-order differential equation, which is basic for our further considerations. If we express the density by the integrated kinetic equation in a way similar to Eq. (5), and apply the Laplace operator to the arising equation, we get

$$\frac{\partial^2}{\partial \mathbf{r}^2} \varrho(\mathbf{r}) = \frac{\gamma}{4\pi v} \int d\Omega \int_0^\infty d\tilde{r} e^{-\tilde{r}} \left(\frac{\partial}{\partial \mathbf{r}} \hat{\mathbf{e}}_\Omega \right) \left(\hat{\mathbf{e}}_\Omega \frac{\partial}{\partial \mathbf{r}} \right) \times \varrho(\mathbf{r} - \tilde{r} \hat{\mathbf{e}}_\Omega). \quad (7)$$

Note that the parts of the Laplace operator corresponding to angular derivatives vanish by the integration over Ω . On the other hand, calculating the source density $(\partial/\partial \mathbf{r})\mathbf{j}(\mathbf{r})$ from Eq. (6) and comparing the result with Eq. (7), we find $(\partial/\partial \mathbf{r})^2 \varrho(\mathbf{r}) = -(\gamma/v^2)(\partial/\partial \mathbf{r})\mathbf{j}(\mathbf{r})$. Since the current is source free, we are left with Laplace's equation,

$$\frac{\partial^2}{\partial \mathbf{r}^2} \varrho(\mathbf{r}) = 0. \quad (8)$$

This is a surprisingly simple relation compared to the generally nonlocal relation between current density and density gradient found in Eq. (6).

If a density $\varrho^s(\mathbf{R})$ is given as a Dirichlet boundary condition on a sphere $\{\mathbf{R}\}$ of radius R centered at the origin, the density which obeys Laplace's equation in the outer region $r \geq R$ can be constructed using the so-called inversion method:¹³

$$\varrho(\mathbf{r}) = \frac{(r^2 - R^2)}{4\pi} \int d\Omega_{\mathbf{R}} \frac{\varrho^s(\mathbf{R})}{(r^2 + R^2 - 2rR \cos \Theta)^{3/2}}, \quad (9)$$

where Θ is the angle between \mathbf{r} and \mathbf{R} .

In the following, we will assume rotational symmetry with respect to the direction $\theta = 0$. This is legitimate for a homogeneous bulk and for a spherically symmetric scatterer to be introduced later on. Under this assumption, the angle-dependent contribution in Eq. (9), which is dominant for $r \gg R$, is the dipole field,

$$\varrho_d(\mathbf{r}) = \frac{3R^2}{2r^2} \cos \theta \int_{-1}^1 d\zeta \zeta \varrho^s(\zeta) \equiv p \frac{\cos \theta}{r^2}, \quad (10)$$

with $\zeta \equiv \cos \theta'$ and the dipole moment $p = 3R^2 \int_{-1}^1 d\zeta \zeta \varrho^s(\zeta)/2$. [The spherically symmetric part of Eq. (9) simply reproduces the equilibrium density and is of no importance here.]

Remember that all preceding formulas were derived for a homogeneous bulk. Let the obstacle now be present around the origin as shown in Fig. 1. Its presence disturbs the homogeneity of the bulk. Then, Eqs. (5)–(8) are valid only if the obstacle is small compared to the MFP, or more precisely, if $(R_{\text{ob}}/l)^3 \ll 1$. This condition ensures that the perturbed region is small compared to the total region, where contributions to the integrals in Eq. (5)–(7) come from.

Our goal is now to calculate the density ϱ^s from the scattered current on the auxiliary sphere $\{\mathbf{R}\}$ of radius R (see Fig. 1). This allows us to obtain the dipole moment in Eq. (10). The dipole is just the RRD introduced by Landauer,¹ which determines the additional resistivity of the obstacle. We characterize the obstacle by a scattering cross section $\sigma(\Theta)$, i.e., the latter depends only on the difference of incidence and scattering solid angles. This ensures the rotational symmetry employed above.

If an angle-dependent current density $j^{\text{inc}}(\Omega)$ is inci-

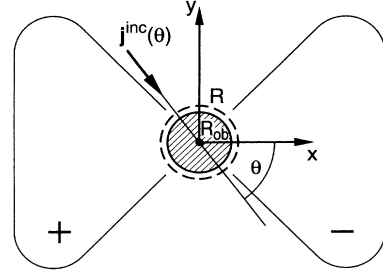


FIG. 1. The spherical obstacle with radius R_{ob} is enclosed by the auxiliary sphere of radius R (dashed). An asymptotic current flowing in the direction $\theta = 0$ induces the density dipole indicated by the large regions labeled + for density excess and – for density deficit. The bold arrow indicates the current density incident on the obstacle at an angle θ . On the auxiliary sphere, the short-range and long-range problems are coupled.

dent on the obstacle centered at the origin, then the radially outgoing current density on a sphere $\{\mathbf{R}\}$ enclosing the obstacle is

$$j^{\text{out}}(\Omega_{\mathbf{R}}) = j^{\text{inc}}(\Omega_{\mathbf{R}}) + \delta j(\Omega_{\mathbf{R}}), \quad (11)$$

$$\delta j(\Omega_{\mathbf{R}}) = \frac{1}{R^2} \int d\Omega' \{ \sigma(\Theta) - \delta(\Theta)\sigma \} j^{\text{inc}}(\Omega'), \quad (12)$$

where Θ is the angle between $\hat{\mathbf{e}}_{\Omega_{\mathbf{R}}}$ and $\hat{\mathbf{e}}_{\Omega'}$. The second term in the brackets takes into account that the current in the forward direction is diminished by the total scattered current. $\delta j(\Omega)$ can be associated with the source term used in Ref. 8 in the context of a Boltzmann approach. It is on the auxiliary sphere where the short-range scattering problem and the long-range diffusion problem are coupled with each other. In order to use a simple relation of the type $\varrho = v^{-1}j$ on the sphere $\{\mathbf{R}\}$, we must take $\delta j(\Omega_{\mathbf{R}})$ in the *quantum-mechanical* far field region. In other words, the radius R of the sphere where δj is taken must be larger than the obstacle by some Fermi wavelengths. First we will discuss the case of $R_{\text{ob}} \gg \lambda$, where $R \approx R_{\text{ob}}$ is a good approximation. In that quantum-mechanical far-field region, the density change on $\{\mathbf{R}\}$ is $\delta \varrho^s(\mathbf{R}) = v^{-1} \delta j(\Omega_{\mathbf{R}})$. In our classical model, we omit all other density contributions of the quantum-mechanical near field. We believe this approximation to be applicable since the quantum-mechanical length scale λ is much smaller than the length scale of the bulk diffusion process. Background scattering and diffusion become important only at distances from the obstacle, where the density can be described well by the quantum-mechanical scattering far field.

In Eq. (12), the incident current depends only on Ω , but not on \mathbf{r} . This is a consequence of the condition $R_{\text{ob}} \ll l$. Otherwise the incident current would vary over the obstacle region. For the calculation of the additional resistivity due to the obstacle, it is sufficient to consider

only the density change $\delta\rho^s(\mathbf{R})$ instead of the total density on the auxiliary sphere.

In Eq. (12), the incident current density plays a central role and is an involved quantity. First, it comprises the primarily incident current density $j^{(0)}(\Omega)$, i.e., the current distribution of the homogeneous unperturbed bulk,

$$j^{(0)}(\Omega) = \text{const} + \frac{3|\mathbf{j}_0|}{4\pi} \cos\theta, \quad (13)$$

where $\theta = 0$ marks the direction of the asymptotic current \mathbf{j}_0 . Second, $j^{\text{inc}}(\Omega)$ contains also contributions which result from multiple backscattering cycles with the surrounding bulk material: Particles once scattered by the obstacle can be scattered by the background and, thus, have a chance to return to the obstacle, forming anew an incident current component. This component can be calculated from the changed density $\delta\rho(\mathbf{r})$ around the obstacle by means of Eq. (5). $\delta\rho(\mathbf{r})$ in turn is determined via Eqs. (9) and (12) by the correct incident current. Thus, we can calculate $j^{\text{inc}}(\Omega)$ self-consistently from the equation

$$j^{\text{inc}}(\Omega) = j^{(0)}(\Omega) + \int_{R_{\text{ob}}}^{\infty} dr \frac{v e^{-\frac{r-R_{\text{ob}}}{l}}}{(4\pi)^2 l} \times \int d\Omega_{\mathbf{R}} \frac{(r^2 - R_{\text{ob}}^2) \delta\rho^s(\mathbf{R})}{(r^2 + R_{\text{ob}}^2 - 2rR_{\text{ob}} \cos\Theta^*)^{3/2}}. \quad (14)$$

Θ^* is the angle between $\hat{\mathbf{e}}_{\Omega_{\mathbf{R}}}$ and $-\hat{\mathbf{e}}_{\Omega}$. Note that particles incident on the scatterer at a direction $\hat{\mathbf{e}}_{\Omega}$ come from a region along the direction $-\hat{\mathbf{e}}_{\Omega}$. The incident currents can be represented by a series of Legendre polynomials,

$$j^{\text{inc}}(\Omega) = \sum_n j_n P_n(\cos\theta). \quad (15)$$

Note again the symmetry with respect to the $\theta = 0$ axis. For the calculation of the RRD, we need only the $n = 1$ term. One easily convinces oneself by using the addition theorem of the spherical harmonics¹³ that there is no coupling between terms belonging to different angular components n in the self-consistency scheme of Eq. (14). This is a peculiarity of our model using a spherically symmetric obstacle where only intervals between solid angles occur. Since the primarily incident current density is proportional to $\cos\theta$ [see Eq. (13)], all relevant quantities in the present problem also show only a $\cos\theta$ dependence.

Then, Eq. (14) can be solved analytically for $n = 1$. The result is

$$j_1 = \frac{3|\mathbf{j}_0|}{4\pi} + \frac{\sigma_T}{2R_{\text{ob}}l} j_1, \quad (16)$$

with the transport cross section $\sigma_T \equiv \int d\theta \sin\theta(1 - \cos\theta)\sigma(\theta)$.

From Eq. (16), we deduce that the scattering strength of the obstacle is enhanced by a factor $(1 - \sigma_T/2R_{\text{ob}}l)^{-1}$. Therefore, we can replace the usual transport cross section by the effective one,

$$\sigma_T \rightarrow \tilde{\sigma}_T = \frac{\sigma_T}{1 - \frac{\sigma_T}{2R_{\text{ob}}l}} \quad (17)$$

and use this quantity in all further calculations. This is the main result of the present paper. The central position of the bulk MFP in our model is underlined by its occurrence in the enhancement factor. The larger the MFP is, the smaller the probability is for higher order scattering cycles to take place. This point has already been made in Ref. 1. However, Landauer predicted a slightly different enhancement factor.

Now we consider briefly the case of an obstacle, which is small compared to the wavelength. Then, the radius R of the sphere on which the quantum-mechanical far field has to be taken, cf. Eq. (12), must be of the order of some wavelengths. Inserting this for R in the subsequent formulas leads, finally, to an enhancement factor, which is approximately $[1 - (\sigma_T/\lambda^2)(\lambda/l)]^{-1}$. Such a correction, however, is definitely beyond the limits of the present quasiclassical model, where λ/l is *a priori* negligible.

III. RESISTIVITY

It is not sensible to attribute a resistance to a single obstacle in the bulk. Therefore, we take a random distribution of obstacles with an effective transport cross section $\tilde{\sigma}_T$ over the entire bulk. Their volume density is \mathcal{N} , which is assumed to be low enough to treat the obstacles as acting independently (i.e., in the dilute limit). Instead of the carrier density, we consider the quantity $u(\mathbf{r}) = \rho(\mathbf{r})/n(E)$, where $n(E) = (m^2 v)/(2\pi^2 \hbar^3)$ is the local density of states. m is the effective carrier mass. In the following, all quantities have to be taken at the Fermi energy, since only those carriers give a contribution to the transport. The difference of $u(\mathbf{r})$ between two points \mathbf{r}_1 and \mathbf{r}_2 , which is additionally introduced by the random distribution of obstacles, is

$$u(\mathbf{r}_1) - u(\mathbf{r}_2) = \frac{2\pi^2 \hbar^3}{m^2 v_F} \sum_i [\varrho_d(\mathbf{r}_1|\mathbf{r}_i) - \varrho_d(\mathbf{r}_2|\mathbf{r}_i)], \quad (18)$$

where $\varrho_d(\mathbf{r}|\mathbf{r}_i)$ is the dipole field of an individual obstacle centered at position \mathbf{r}_i , see Eq. (10). v_F is the Fermi velocity. After a configurational average with respect to the scatterer positions, we get

$$\langle u(\mathbf{r}_1) - u(\mathbf{r}_2) \rangle = \frac{12\pi^3 \hbar^3}{m^2 v_F^2} (x_2 - x_1) \mathcal{N} \tilde{\sigma}_T |\mathbf{j}|. \quad (19)$$

Thus, $\langle u(\mathbf{r}_1) - u(\mathbf{r}_2) \rangle$ does not depend on the coordinates perpendicular to the asymptotic current direction. Now it makes sense to identify this quantity with the additional potential drop $e\delta U$ over the distance $x_2 - x_1$, due to the obstacle distribution. Hence, we find the additional resistivity,

$$\delta\rho = \frac{12\pi^3 \hbar^3}{m^2 v_F^2 e^2} \mathcal{N} \tilde{\sigma}_T. \quad (20)$$

The scattering cross section σ_T enters the resistivity

via $\tilde{\sigma}_T$ in a nonlinear manner. This was predicted from the very beginning of the RRD concept, see Refs. 1 and 6. Here we have confirmed this prediction.

IV. SUMMARY

In conclusion, we have derived an analytical expression of the RRD for a spherically symmetric obstacle, which is small compared to the bulk MFP. This was done within a classical framework starting from a local kinetic equation. The near and far fields of the density were treated separately. The current density incident on the obstacle turned out to be a central quantity. We have shown how to calculate it self-consistently. Finally, we have found the additional resistivity, which is introduced by a random distribution of obstacles in the dilute limit.

Our main result is that the impurity scattering cross section enters the resistivity in a nonlinear fashion even in the three-dimensional case, as predicted by Landauer in 1957. This nonlinearity should be experimentally accessible if pure bulk samples are doped with impurities, whose average scattering cross section and size are well defined and can be varied over a wide range.

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