Exact scattering theory for the Landauer residual-resistivity dipole

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An exact-scattering-theory calculation for the density of electrons around localized impurities in bulk metals for arbitrary transport current is performed within the noninteracting-Fermi-gas approximation. To first order in the transport current, one recovers the Landauer residual-resistivity dipole plus additional Friedel oscillations. Numerical calculations for the density at arbitrary currents are performed for the one-, two-, and three-dimensional case.

I. INTRODUCTION

The distortion of the electronic density by a localized static impurity in a metal is a classic subject in solid-state theory and leads to the well-known Friedel oscillations associated with the sharpness of the Fermi distribution at zero temperature.¹ In the case of a metal with a finite transport current density j = nev, the related question has been addressed in a classic paper by Landauer.² Landauer argued that with carriers impinging on one side of a potential barrier there will be corresponding depletion on the other side, resulting in a dipolar density and potential distribution. This so-called residual-resistivity dipole^{3,4} is considered as the ultimate source of resistance in a disordered metal and leads to a highly inhomogeneous distribution of density and electric field for each specific sample which is absent in theories where an average over the impurity distribution is taken. In order to determine the dipole strength p of the associated electrostatic potential $p \cos\theta/r^2$ (in three dimensions), Landauer³ argued that the average electric polarization field $E = 4\pi n_i p$ for an impurity density n_i which is small enough that the individual scatterers may be considered as independent must be equal to the field $E = \rho j$ associated with a given current density j by Ohm's law. Since the residual resistivity ρ is given by $\rho = m/ne^2 \tau_{\rm tr}$, with $1/\tau_{\rm tr} = n_i v_F \sigma_{\rm tr}$ and $\sigma_{\rm tr} = \int d\Omega (1 - \cos\theta) \sigma(\theta)$, the transport cross section due to a single impurity, one obtains^{3,4}

$$p = \frac{\hbar k_F v}{4\pi e} \sigma_{\rm tr} \quad \text{for } d = 3 , \qquad (1)$$

with v the transport velocity. As emphasized by Landauer³ the dipole strength p is proportional to the scattering cross section and thus (at least) quadratic in the impurity potential. As a consequence first-order perturbation theory is inadequate for a proper treatment of this problem. Microscopic derivations of the Landauer resistivity dipole usually start from calculating the change in the electronic momentum distribution δf_k to first order in the *averaged* electric field using the Boltzmann equation. Integrating this with the probability density $|\Psi_k(\mathbf{x})|^2$ of the impurity-scattering states then gives the local change $\delta n(\mathbf{x})$ in density associated with a finite transport current.^{4,5} Within the Thomas-Fermi approximation for screening, a given $\delta n(\mathbf{x})$ translates into a local electrostatic potential of the form

$$\delta\phi(\mathbf{x}) = \frac{1}{e} \frac{d\mu}{dn} \delta n(\mathbf{x})$$

where the thermodynamic derivative $d\mu/dn$ is equal to the inverse density of states at the Fermi energy.

Our aim in the present work is to give a very simple pure-scattering-theory calculation of the local density around an impurity which is valid for arbitrary large transport current j. It contains the Landauer residualresistivity dipole as the linear term in an expansion in powers of *j*. In addition to the smooth dipolar distribution, however, we find dynamic Friedel-type oscillations which, except for very large distances, decay with the same power as the dipolar term. Such oscillations have been previously mentioned by Schaich⁵ and their importance for the so-called phase-sensitive voltage measurements in a one-dimensional geometry was recently discussed by Büttiker.⁶ Here we will perform detailed numerical calculations for the full densities around a localized impurity in one, two, and three dimensions using simple model potentials. Moreover, in view of the recent direct observation of the potential distribution at grain boundaries in a thin-metal film with a tunneling microscope, 7 we have included a calculation of the electronic density in two dimensions with extended one-dimensional scatterers.

II. ELECTRON DENSITY AT ARBITRARY TRANSPORT CURRENT

A. General results

We consider a noninteracting Fermi gas with the unperturbed Hamiltonian H_0 . Its eigenstates are Slater determinants of one-electron plane-wave states $|\mathbf{k}\rangle$ with single-particle energy $\varepsilon_{\mathbf{k}} = (\hbar \mathbf{k})^2 / 2m$. In the presence of a local scattering center at the origin characterized by a potential $V(\mathbf{x})$, a complete set of one-particle eigenstates of the full Hamiltonian H are the outgoing scattering states $|\mathbf{k}, +\rangle$ [we assume, for simplicity, that there are no bound states in $V(\mathbf{x})$]. The states $|\mathbf{k}, +\rangle$ may be obtained by solving the corresponding stationary oneparticle Schrödinger equation in $V(\mathbf{x})$ and are assumed to be known. A situation with a finite transport current $\mathbf{j}=ne\mathbf{v}$ is now set up by assuming that an incoming initial state with plane-wave occupation numbers $f(\varepsilon_{\mathbf{k}-mv\hbar})$ is scattered at the impurity. Here $f(\varepsilon_{\mathbf{k}})=(e^{\beta(\varepsilon_{\mathbf{k}}-\mu)}+1)^{-1}$ is the usual Fermi function with chemical potential μ . The momentum distribution for a current carrying situation is thus simply a shifted Fermi sphere. The corresponding density is then given by

$$n(\mathbf{x}) = \int \frac{d^d k}{(2\pi)^d} f(\varepsilon_{\mathbf{k}-m\mathbf{v}/\hbar}) |\langle \mathbf{x} | \mathbf{k}, + \rangle|^2 .$$
 (2)

This result is just a simple generalization of the static Friedel expression at vanishing transport current j=0. A detailed formal derivation in the context of the related problem of a particle which is dragged through a Fermi gas with fixed velocity v was recently given by two of the present authors.^{8,9} Expanding (2) to linear order in v and assuming zero temperature T=0 for simplicity, we obtain a correction to $n(\mathbf{x})$ at $\mathbf{v}=\mathbf{0}$ of the form $[k=|\mathbf{k}|$, here $d \ge 2$; for one dimension see Eq. (7) below]

$$\delta n\left(\mathbf{x}\right) = \frac{m}{\hbar k_F} \int \frac{d^d k}{(2\pi)^d} \mathbf{v} \cdot \mathbf{k} |\Psi_{\mathbf{k}}(\mathbf{x})|^2 \delta(k - k_F) + O(v^2) , \qquad (3)$$

which, as we will see, gives rise to the Landauerresidual-resistivity dipole. Numerically it turns out that the terms in (3) which are quadratic or higher order in vare negligible for transport velocities v smaller than about $0.05v_F$. In the limit of very large velocities $v \gg \max(v_F, v_T)$ with $v_T = (T/m)^{1/2}$, as the thermal electron velocity the factor $|\Psi_k(x)|^2$ taken at $\mathbf{k} = \mathbf{k}_v = m\mathbf{v}/\hbar$ may be removed from the integral. Then using

$$\int \frac{d^d k}{(2\pi)^d} f(\varepsilon_{\mathbf{k}-\mathbf{k}_v}) = n ,$$

we obtain

$$\lim_{v > \max\{v_F, v_T\}} n(\mathbf{x}) = n |\Psi_{\mathbf{k}_v}(\mathbf{x})|^2 .$$
(4)

Obviously, in this limit the Fermi statistics no longer plays any role. In the following we will evaluate the general result (2) numerically at T=0 for simple model potentials in one, two, and three dimensions.

B. One dimension

For this case the density has been calculated explicitly in Appendix C of Ref. 9 with the result

$$n(x) - n = \begin{cases} \int_{k_F - k_v}^{k_F + k_v} \frac{dk}{2\pi} R(k) + \int_0^{k_F + k_v} \frac{dk}{\pi} R^{1/2}(k) \cos(2kx - \alpha_k), & x < -a \\ - \int_{k_F - k_v}^{k_F + k_v} \frac{dk}{2\pi} R(k) + \int_0^{k_F - k_v} \frac{dk}{\pi} R^{1/2}(k) \cos(2kx - \tilde{\alpha}_k), & x > a \end{cases},$$
(5)

valid for $v < v_F$. Here R(k) is the reflection probability at the corresponding potential which we assume to be concentrated on |x| < a while α_k or $\tilde{\alpha}_k$ are the phases of the reflection amplitude for scattering from left or right. For vanishing transport current (5) leads to static Friedel oscillations of the form

$$\lim_{|x| \to \infty} n(x)|_{v=0} = n + R^{1/2} \frac{\sin(2k_F x - \tilde{\alpha}_{k_F})}{2\pi x} , \quad (6)$$

which decay like 1/x. Here and in the following we have set $R(k_F)=R$. Also we have used that R(k=0)=1 and $(\tilde{\alpha})_{k=0}=\pi$ quite generally. To linear order in j we find from (5) an additional contribution $(n=k_F/\pi)$

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$$\delta n(x) = n \frac{v}{v_F} \times \begin{cases} R + R^{1/2} \cos(2k_F x - \alpha_{k_F}), & x < -a \\ -R - R^{1/2} \cos(2k_F x - \widetilde{\alpha}_{k_F}), & x > a \end{cases}$$
(7)

This shows that in one dimension the Landauer residualresistivity dipole corresponds to a jump of the average density $\Delta n = 2nRv / v_F$ across a single scatterer corresponding to a "dipole strength"

$$p = \frac{\hbar k_F v}{e} R \quad \text{for } d = 1 .$$
 (8)

In addition, there are oscillatory contributions proportional to $R^{1/2}$. These terms have become relevant recently in the context of mesoscopic systems. Indeed it has been shown by Büttiker⁶ that in a single-channel transmission problem the root-mean-square fluctuations of the resistance at fixed current j may be large compared with the fundamental value h/e^2 in the limit $R \rightarrow 1$, provided that the voltage measurement is sensitive to the potential fluctuations associated with (7). It should be pointed out that the exact expression (5) shows that the oscillations asymptotically always decay like 1/x for arbitrary v as in the case v=0 while (7) is valid only as long as $k_F|x| \ll v_F/v$. A similar situation arises in dimensions d=2 and 3 (see below) which shows that the expansion (3) in powers of v is not uniformly convergent. For large velocities $v >> v_F$ we use (4) to obtain

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$$\lim_{v \to v_F} n(x) = n \times \begin{cases} 1 + R(k_v) + 2R^{1/2}(k_v)\cos(2k_v x - \alpha_{k_v}) \\ x < -a \qquad (9) \end{cases}$$

with T=1-R being the transmission probability. It is interesting to note that after averaging the oscillatory components and neglecting the energy dependence of R(k) and T(k), the result (9) corresponds to the naive picture of the density in front or behind a barrier which is sometimes used in elementary derivations of the Landauer formula $g = (e^2/h)T/R$ for the conductance of a one-dimensional channel with transmission probability T(see the discussion in Sec. III below).

C. Two dimensions

Scattering theory in two dimensions has some peculiar properties and we will follow the notation used by Adhikari.¹⁰ The asymptotic behavior of the scattered wave function with an incoming wave in the x direction is $(k \equiv k_x > 0)$

$$\Psi_k(\mathbf{x}) \sim e^{ikx} + \left[\frac{i}{k}\right]^{1/2} f_k(\theta) \frac{e^{ikr}}{\sqrt{r}} \text{ as } r \to \infty .$$
 (10)

It defines a dimensionless scattering amplitude $f_k(\theta)$ which determines the differential cross section $\sigma(\theta)$ by $\sigma(\theta) = |f_k(\theta)|^2 / k$. In the limit $kr \to \infty$ the incoming plane wave can formally be written as

$$\lim_{kr \to \infty} e^{i\mathbf{k} \cdot \mathbf{x}} = \left[\frac{2\pi}{kr}\right]^{1/2} \left[e^{i(kr - \pi/4)}\delta(\Omega_k - \Omega_x) + e^{-i(kr - \pi/4)}\delta(\Omega_k + \Omega_x)\right],$$
(11)

which follows from decomposing $e^{i\mathbf{k}\cdot\mathbf{x}}$ into partial waves¹⁰ using the asymptotic behavior of the associated Bessel functions and the Poisson summation formula. Using this and the optical theorem

$$\sigma_{\rm tot} = \frac{2\sqrt{2\pi}}{k} {\rm Im} f_k(0) ,$$

the asymptotic behavior of the square of the scattering wave function reads

$$\lim_{kr \to \infty} |\Psi_k(\mathbf{x})|^2 = 1 - \frac{\sigma_{\text{tot}}}{r} \delta(\Omega_k - \Omega_x) + \frac{\sigma(\theta)}{r} + \frac{2\sqrt{2\pi}}{kr} \operatorname{Re}[f_k(\pi)e^{2ikr}]\delta(\Omega_k + \Omega_x) .$$
(12)

We emphasize that (12) and the corresponding result (17) in the three-dimensional case below can only be used in the distribution theory sense after integrating over k, otherwise terms of order 1/r should already have been included in (10). At vanishing transport current j=0 the

asymptotic behavior of the density (2) at T=0 is therefore given by $[\alpha_k = \arg f_k(\pi)]$

$$\lim_{t \to \infty} n(\mathbf{x}) = n + \frac{\sqrt{2\pi}}{(2\pi r)^2} |f_{k_F}(\pi)| \sin(2k_F r + \alpha_{k_F}) .$$
(13)

The static Friedel oscillations are thus again proportional to the backscattering amplitude but decay as $1/r^2$ in two dimensions. Here we have used that f_k vanishes at k=0. To linear order in j we find from (3) that

$$\lim_{r \to \infty} \delta n(\mathbf{x}) = -n \frac{\mathbf{v} \cdot \hat{\mathbf{x}}}{\pi v_F r} \left[\sigma_{\mathrm{tr}} + \frac{2\sqrt{2\pi}}{k_F} \mathrm{Re}[f_{k_F}(\pi) e^{i2k_F r}] \right]$$
(14)

with the usual transport cross section $\sigma_{tr} = \int d\theta (1 - \cos\theta)\sigma(\theta)$ at the Fermi energy and $\hat{\mathbf{x}}$ as the unit vector in the x direction. The first nonoscillating term in (14) is precisely the Landauer residual-resistivity dipole in two dimensions. Defining its strength p via

$$\delta n\left(\mathbf{x}\right) = -e\frac{dn}{d\mu}\frac{p\widehat{\mathbf{v}}\cdot\widehat{\mathbf{x}}}{r}$$

we have

$$p = \frac{\hbar k_F v}{2\pi e} \sigma_{\rm tr} \quad \text{for } d = 2 , \qquad (15)$$

a result which is equivalent to that given by Sorbello and Chu.⁴ In addition to the dipole contribution, however, there is a Friedel-like oscillating term with wave vector $2k_F$ and strength $f_{k_F}(\pi)$, similar to the static result Eq. (13) but decaying as 1/r instead of $1/r^2$. Again, as in the case of one dimension, the 1/r decay of the oscillating term is restricted to $k_F r \ll v_F / v$ and is asymptotically replaced by a $1/r^2$ behavior. Nevertheless for not too large distances this term makes a noticeable contribution to the complete density. An example for the spatial dependence of the density in the case of a hard-disk potential of radius a which is based on a detailed numerical evaluation of (2) with the exactly known scattering wave functions is shown in Fig. 1. Clearly the Friedel oscillations on top of the dipole term are rather pronounced. Moreover, there

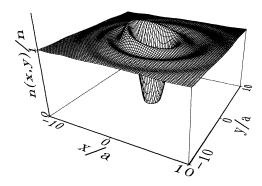


FIG. 1. Normalized density around a two-dimensional hard disk with $k_F a=1$, $v/v_F=0.2$, and v pointing in the positive x direction.

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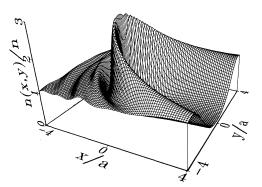


FIG. 2 The same as in Fig. 1 but with $v/v_F = 3$.

is a Doppler shift of the oscillations whose wavelength is shorter in front of than behind the scattering center. This feature is much more pronounced in the case of a very large transport velocity which is shown in Fig. 2 and where essentially the simple asymptotic result (4) applies. There are now huge oscillations in front of the impurity which are caused by the interference between incoming and reflected waves and whose wavelength is no longer related to the Fermi wavelength. In addition there is a deep shadow with almost vanishing density just behind the impurity. Clearly for metals the transport velocity vis always very small compared with v_F ; however, for degenerate semiconductors with low carrier density n it may be possible to realize situations in which v/v_F is no longer small compared with 1.

Finally we want to discuss the case of extended defects in two dimensions which may model grain boundaries, for instance. Indeed these were the relevant scatterers in the experiments by Kirtley, Washburn, and Brady⁷ who did observe that the local potential varies strongly in the vicinity of the grain boundaries. Assuming that the scattering potential is a straight one-dimensional strip V(x,y)=V(x), the Schrödinger equation is effectively one dimensional since the wave function in the y direction is a plane wave. At T=0 the Fermi function places a restriction on k such that $(\mathbf{k}-\mathbf{k}_v)^2 \le k_F^2$, and with $|\Psi_{\mathbf{k}}(\mathbf{x})|^2$ independent of k_y and y the problem reduces to a purely one-dimensional one of the form $(k = k_x)$

$$n(x) = \int_{-k_F + k_{v_x}}^{k_F + k_{v_x}} \frac{dk}{2\pi^2} \left[k_F^2 - \left[k - \frac{mv_x}{\hbar} \right]^2 \right]^{1/2} |\Psi_k(x)|^2 ,$$
(16)

with $\Psi_k(x)$ the scattering states in the one-dimensional potential V(x). Choosing V(x) as a δ -function potential with a reflection probability R=0.9 (i.e., close to one that may be a reasonable description of the experimental situation in Ref. 7) and a velocity $v/v_F=0.1$ in the x direction, we obtain a density distribution as shown in Fig. 3.

We mention that in the presence of an extended defect in two dimensions, the asymptotic value of the density $n(x \rightarrow \pm \infty)$ is not equal to its equilibrium value *n* if *v* is nonzero. Similar to the situation in one dimension, it differs from *n* by a finite, nonzero amount which becomes

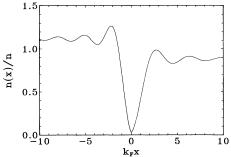


FIG. 3. Normalized density around an extended strip in two dimensions with R=0.9 and $v/v_F=0.1$.

 $\pm nRv/v_F$ in the limit $v \ll v_F$. The Friedel oscillations, however, asymptotically decay like $1/|x|^{3/2}$, formally appropriate for a $1\frac{1}{2}$ -dimensional system.

D. Three dimensions

In three dimensions, with the standard definitions of the scattering amplitude $f_k(\theta)$ and the differential cross section $\sigma(\theta) = |f_k(\theta)|^2$, the asymptotic behavior of $|\Psi_{\mathbf{k}}(\mathbf{x})|^2$ is given by $(k \equiv |\mathbf{k}|)$

$$\lim_{kr \to \infty} |\Psi_{\mathbf{k}}(\mathbf{x})|^{2} = 1 - \frac{\sigma_{\text{tot}}}{r^{2}} \delta(\Omega_{k} - \Omega_{x}) + \frac{4\pi}{kr^{2}} \text{Im}[f_{k}(\pi)e^{2ikr}] \delta(\Omega_{k} + \Omega_{x}) + \frac{\sigma(\theta)}{r^{2}}.$$
(17)

The static, i.e., v=0, Friedel oscillations thus have the standard form

$$\lim_{r \to \infty} n(\mathbf{x}) = n - \frac{|f_{k_F}(\pi)|k_F}{4\pi^2 r^3} \cos(2k_F r + \alpha_{k_F})$$
(18)

decaying like $1/r^3$. The correction to this result to first

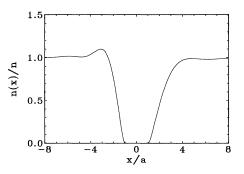


FIG. 4. Normalized density around a hard sphere in three dimension in the forward and backward direction with $k_F a=1$ and $v/v_F=0.2$.

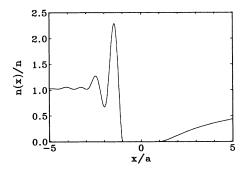


FIG. 5. The same as in Fig. 4 but with $v/v_F = 3$.

order in the transport current j is, according to (3), given by

$$\lim_{r \to \infty} \delta n(\mathbf{x}) = -n \frac{\mathbf{v} \cdot \hat{\mathbf{x}}}{\frac{4}{3} \pi v_F r^2} \times \left[\sigma_{\mathrm{tr}} + \frac{4\pi}{k_F} \mathrm{Im}[f_{k_F}(\pi) e^{i2k_F r}] \right].$$
(19)

Again as in (14) the first term gives the Landauer residual-resistivity dipole with a strength p which is exactly identical to the one which follows from the simple consideration in (1). The oscillatory contribution decays as $1/r^2$ but asymptotically will decay like $1/r^3$ so that the dipole is indeed the dominant term. It is interesting to note that the Landauer residual-resistivity dipole contribution $\delta n(\mathbf{x})$, which is linear in \mathbf{v} but quadratic in the scattering potential, also determines the long-distance behavior of the electronic backflow current $\delta \mathbf{j}$, which, at T=0, has the simple form

$$\delta \mathbf{j}(\mathbf{x}) = v_F \,\delta n(\mathbf{x}) \hat{\mathbf{x}} \,, \tag{20}$$

i.e., it is purely radial and decays as $1/r^2$. As discussed in Ref. 9 this contribution always dominates the dipolar backflow obtained by using linear response in the scattering potential.¹¹ For the case of a hard-sphere potential with radius *a* such that $k_F a=1$, the full normalized density n(x)/n in the direction of the transport current is shown in Figs. 4 and 5 for $v/v_F=0.2$ and $v/v_F=3$, respectively.

III. DISCUSSION

We have performed a simple scattering-theory calculation of the local electronic density at T=0 around impurities at arbitrary transport current and have provided detailed numerical results for the full density at all distances The motivation for dealing with this simple problem in elementary quantum mechanics is due to the fact that it has recently been possible to observe local-potential variations around defects directly with a tunneling microscope.^{7,12} In order to compare the present results with experiment, it is necessary to ensure that one is really measuring the local potential in the vicinity of an impuri-

ty, undisturbed by contact potentials, etc., a point which has been stressed by Büttiker⁶ and Landauer.^{13,14} In this context it is clear that our Thomas-Fermi approximation for screening, where the local electrochemical potential $\delta\mu(x)$ is simply proportional to $\delta n(x)$, misses some of the details of the precise distribution. However, as long as the resolution of the tunneling microscope is not significantly smaller than the screening length, deviations from our simple approach compared to one in which a more refined wave-vector-dependent dielectric constant is used should be irrelevant. Moreover, this assumption also guarantees local charge neutrality on the scale of interest and thus the equality between the electrostatic and the electrochemical potential.¹³ It should also be pointed out that we have not included inelastic effects, which probably will smooth out finer details of the density variation. A similar effect arises from the thermal smearing of the Fermi distribution in (2) which leads to an exponential damping of the $2k_F$ oscillations in the form $\exp[-b(T/T_F)k_Fr]$ with b a constant of order unity. Since direct measurements of the local potential around localized impurities are feasible with the present resolution, we believe that at least the qualitative features of the inhomogeneous density distribution obtained here should be observable in experiment.

Finally we would like to make a few remarks on the relation between the residual-resistivity dipole and calculations of the conductance. In the Landauer approach an incident flux rather than an electric field is the starting point of a calculation of the conductance and the response is a drop in potential rather than a current. In one dimension (7) gives an average potential drop $\Delta \mu = 4\mu (v/v_F)R$ across a single scatterer with the reflection coefficient R. Thus the conductance associated with a single localized impurity is $g = e_j / \Delta \mu = e^2 / hR$. In order to obtain the Landauer result with a factor $T_{\rm tot}/R_{\rm tot}$ for a succession of random scatters with total transmission T_{tot} it is necessary to sum up repeated incidences on a single scatterer in the form $R + R^2 + \cdots = R/(1-R)$ (Refs. 2 and 3) which eventually leads to localization in one dimension. In two and three dimensions the inclusion of multiple scattering within this approach has not been possible yet and the arguments leading to (1) just give the Boltzmann value for the resistivity $\rho = m / ne^2 \tau_{\rm tr}$ consistent with the assumption of independent-scattering processes. Finally we would like to point out that the resistivity ρ as a measure of dissipation in a model with purely elastic scattering arises naturally by viewing the Fermi gas at rest, but dragging the impurities through it with a given velocity v. The associated electronic friction $problem^{8,9}$ then leads to a dissipated power $\Delta \dot{\epsilon} = \eta v^2$ per impurity through the excitation of particle-hole pairs with a fric-tion constant $\eta = mn\sigma_{tr}v_F$.¹⁵ Equating the generated power per volume $n_i \Delta \dot{\varepsilon}$ with ρj^2 leads again to the usual Boltzmann value for ρ . This point of view makes clear that the dissipated power associated with the residual resistance leads to a continuous heating up of the electrons and thus to an increase in their effective temperature¹⁶ unless other degrees of freedom can absorb the energy.

Note added. After submission of the present paper we became aware of a related general work on the resistivity dipole by R. Lenk, Phys. Status Solidi B 155, 627 (1989) and also of recent publications on the specific questions related to the experiments in Ref. 7 by J. P. Pelz and R. H. Koch, Phys. Rev. B 41, 1212 (1990) and by C. S. Chu and R. S. Sorbello, *ibid.* 42, 4928 (1990).

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