Residual-resistivity dipole in electron transport and electromigration

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The structure of Landauer's residual-resistivity dipole is investigated using expressions which have been recently derived from linear-response theory. We calculate the local field and charge density near an impurity in a current-carrying metal. The impurity is assumed to be an isotropic scatterer and is described by an s-wave phase shift. We find that the long-range average field of the residual-resistivity dipole is exactly as obtained by Landauer in a semiclassical picture; i.e., the dipoles give the macroscopic field which drives the current past the scatterers. The charge distribution is not strongly localized, but has important Friedel oscillations extending far from the impurity. Our results are applied to the calculation of the electromigration driving force on a weak scatterer due to the presence of an s-wave scatterer in its vicinity. When the s-wave scatterer is strong, the residual-resistivity dipole contributes substantially to the force on the weak scatterer. Such contributions have not been previously considered in explicit calculations of scattering interference effects in electromigration.

I. INTRODUCTION

The residual-resistivity dipole (RRD) is a fundamental object in the theory of electronic conduction. Introduced into the theory by Landauer in 1957, the RRD is the microscopic source of the electric field which must be set up in a conducting solid in order to drive current past a region containing impurities. Despite its central importance, the RRD has been generally ignored in theoretical descriptions of electron transport. One usually assumes that the macroscopic electric field arises from sources external to the system. In reality, the field has internal sources in the form of dipolar charge distributions localized around each impurity. These are the RRD's. Analyses of electrical resistivity based on the RRD picture have not given any new answers for the resistivity; RRD's have thus far been of conceptual value rather than practical value. As Landauer has pointed out, however, a correct picture of the local dipole field would be helpful in formulating a theory for scattering by inhomogeneities which are neither macroscopic nor point-defect-like. This alone would provide motivation for studying the RRD. Further, if one is interested in the detailed nature of the local field in electrical conductivity, the field of the RRD must be considered. Since the local field acts as the driving force on an ion in a solid, one finds the RRD mentioned in recent theoretical papers on electromigration, which is the phenomenon of ion transport in the presence of an electron current.

A review of the RRD with special emphasis on electromigration has been given by Landauer and Woo. In summary, Landauer found that around each impurity in a conducting solid there forms a localized dipolar charge distribution which he called the RRD. If one denotes the dipole moment of an RRD by \(\vec{P}_0\), then the average field generated by these RRD's in a rectangular sample is given by \(-4\pi N\vec{P}_0\), where \(N\) is the number of impurities per unit volume. When the value of \(\vec{P}_0\) calculated by Landauer is used in this expression, there results precisely the average additional field needed to drive a current past these impurities in the first place. Thus, there is no true external charge which sets up the additional field; the field arises instead from the RRD charge distributions. It was further argued by Landauer and Woo that the RRD is localized to within a screening length from the impurity. This strong localization led them to predict a large RRD force on the impurity.

Up to now there have not been any explicit calculations of the RRD charge or the RRD field. Local-field calculations have been made within quantum-mechanical formalism and semiclassical formalism. These calculations went only to terms linear in the impurity potential \(V\). Since the RRD is proportional to the cross section, it will not show up unless the calculations are pushed to second order in \(V\).

One reason for the lack of activity in calculating RRD fields is obviously the extra work required to go to the next order in perturbation theory. Moreover, if one is interested only in the force on an ion in electromigration one need not explicitly examine the RRD. Instead, it turns out that one can calculate the force to all orders in \(V\) if one takes the lowest-order perturbation-theory expression for the force and replaces \(V\) by the \(T\) matrix for the impurity. This procedure is valid for isolated impurities; for more complicated scatterers, the force can also be expressed in terms of \(T\) matrices. Thus, the RRD need not be explicitly singled out in calculating electromigration...
migration forces. Nonetheless, from a fundamental point of view, it is desirable to investigate the local RRD field near an impurity. Besides illuminating some hidden assumptions in transport theory, such an investigation will clarify the picture of Landauer and Woo for electromigration and other transport phenomena.4,5

In this paper we present an explicit calculation of the RRD charge density and the associated local electric field around an impurity in a jellium background. The calculation is performed for an impurity which is predominantly an s-wave scatterer. Calculation of the local field is formally equivalent to determining the force on a weak scatterer in the vicinity of the impurity. Our results will thus be immediately applicable to the problem of determining the electromigration force on a weak scatterer due to interference effects caused by the presence of a strong s-wave scatterer in its neighborhood. No explicit calculation of interference effects in electromigration has appeared in the literature except for the case of only weak scatterers.16 In a study of liquid metals we again used weak-scattering expressions, but followed heuristic arguments to replace $V$ by the $T$ matrix. These procedures, as we discuss in Sec. IV, systematically discard RRD contributions. As a result of the present study we can estimate the errors involved.

As far as the structure of the RRD is concerned, we shall see that the long-range dipole field of the RRD is precisely as described by Landauer.1 However, the actual charge distribution of the RRD is not so localized as assumed by Landauer and Woo.8 Instead, we find the RRD extends over a large region where it is inextricably intertwined with Friedel oscillations.

II. LOCAL FIELDS AND CHARGE DENSITIES

We wish to obtain the response of an electron gas to an impurity in the presence of an applied electric field. The Kubo linear-response formalism has been applied to this problem18 and has led to a better picture of the local fields and charge densities around the impurity.5,7,11,16-20 For an impurity in jellium all of the linear-response results agree with each other and with Liouville-equation calculations in the relaxation-time approximation4,11 in the regime $k_F l \gg 1$, where $k_F$ is the Fermi wave vector and $l$ is the mean free path.21 This $k_F l \gg 1$ regime is the regime of physical interest for metals describable within a jellium model.

The diagrammatic Green’s-function calculation of Sham7 was the most general of the first linear-response calculations in that it explicitly included electron screening and strong scattering by the impurity. Further studies based on the diagrammatic technique have also been made.11,13,20

Within an independent-particle approximation these analyses lead to the physically appealing result that the local electron density $n_0(\mathbf{r})$ around an impurity can be obtained by simply populating the electron scattering states $\psi_\mathbf{k}(\mathbf{r})$ according to the distribution function $g_\mathbf{k}$ appropriate to the electron-transport problem. This result is explicitly derived by Schaich8 and is also implicit in Sham’s analysis.7 The expression for the density is

$$n_0(\mathbf{r}) = \sum_k g_\mathbf{k} |\psi_\mathbf{k}(\mathbf{r})|^2,$$

where the sum is over all states $\mathbf{k}$ and where $g_\mathbf{k}$ is the solution of the Boltzmann equation, namely

$$g_\mathbf{k} = -\tau e \mathbf{v}_\mathbf{k} \cdot \mathbf{E}_0 \delta (\epsilon_\mathbf{k} - \epsilon_p).$$

Here $\tau$ is the relaxation time, $e$ is the charge of the proton, $\mathbf{v}_\mathbf{k}$ is the electron velocity, and $\mathbf{E}_0$ is the macroscopic electric field. The Fermi energy is denoted by $\epsilon_p$ and the energy of the state $\mathbf{k}$ is $\epsilon_\mathbf{k} = \hbar^2 k^2/2m$, where $m$ is the electron mass. The wave function $\psi_\mathbf{k}(\mathbf{r})$ evolves from an incoming plane wave $\exp(i \mathbf{k} \cdot \mathbf{r})/\Omega^{1/2}$, where $\Omega$ is the crystal volume. In our model the electron propagates as a free particle, except for its interaction with the impurity. Equation (1) is of the form assumed by Bosvieux-Friedel14 for the “dynamic polarization” due to the electron current, i.e., the “electron wind” effect. This has been pointed out by Schaich.

When the independent-particle picture is generalized to include a self-consistent treatment of the electron-electron interaction, the electron density is no longer given by Eq. (1). If screening is considered within the random-phase approximation (RPA) or, more generally, if local linear screening is assumed, one can show that the true density is not given by Eq. (1), but rather by

$$n(\mathbf{r}) = n_0(\mathbf{r}) + n_\infty(\mathbf{r}),$$

where $n$ is the true density and $n_\infty$ is the screening density. The Fourier transform of $n_\infty$ is related to $n_0$ according to the linear relation20,23

$$n(\mathbf{q}) = \frac{n_0(\mathbf{q})}{\epsilon(q)},$$

where $\epsilon(q)$ is the dielectric function and will be assumed to be that given within the RPA.

The force $\mathbf{F}$ exerted on an ion, or any object which interacts with the electrons, can be written in the form4,16

$$\mathbf{F} = -\int n(\mathbf{r}) \frac{\partial \nu_0(\mathbf{r})}{\partial \mathbf{R}} d^3r,$$
where $R$ is the position of the ion and $v_0(\mathbf{F} - \mathbf{R})$ is the bare potential which describes the interaction of the electrons with the ion of interest. In Eq. (5) we are only considering the force arising from the local electron response $n_0(\mathbf{F})$. The force exerted by the macroscopic field $\mathbf{E}_\infty$ can be added separately as $Ze \mathbf{E}_\infty$, where $Ze$ is the charge of the ion. We are not concerned with this direct force here so we shall ignore it.

Using expression (4) one can transform Eq. (5) into the alternate form\textsuperscript{23}

$$
\mathbf{F} = \int n_0(\mathbf{F}) \frac{\partial v(\mathbf{F} - \mathbf{R})}{\partial \mathbf{F}} \, d^3 \mathbf{F},
$$

(6)

where $v$ is the screened potential. The Fourier transforms of $v(\mathbf{F})$ and $v_0(\mathbf{F})$ are related by the dielectric function, i.e., $v(\mathbf{q}) = v_0(\mathbf{q})/\epsilon(q)$.

The local electric field, which we denote by $\mathbf{E}_L$, can be immediately obtained by applying Eq. (6) to find the force on a test charge $Q$ at position $\mathbf{R}$\textsuperscript{5}. Taking the limit of $\mathbf{F}/Q$ as $Q \to 0$, this gives for the local field at position $\mathbf{R}$ the result

$$
\mathbf{E}_L(\mathbf{R}) = \int n_0(\mathbf{F}) \frac{\partial \phi(\mathbf{F} - \mathbf{R})}{\partial \mathbf{F}} \, d^3 \mathbf{F},
$$

(7)

where $\phi$ is the screened electrical potential. Within the RPA the transform of $\phi(\mathbf{F})$ is given by $\phi(\mathbf{q}) = -4\pi e/\mathbf{q}^2 \epsilon(q)$. The total field at $\mathbf{R}$ is the sum of $\mathbf{E}_L$ and the applied field $\mathbf{E}_\infty$.

### III. MODEL CALCULATION

We consider the charge distribution around a highly-localized spherically symmetric impurity potential. The scattering wave functions can be expanded in partial waves and written in the form\textsuperscript{24}

$$
\psi(\mathbf{F}) = \frac{1}{\Omega_1^{1/2}} \left[ e^{i \mathbf{F} \cdot \mathbf{R}} + \sum_{j=0} \frac{(2l+1)}{\mathbf{l}+1} P_l(\mathbf{k} \cdot \mathbf{R}) \right] \times \left[ R_l(\mathbf{r}) - j_l(\mathbf{k} \mathbf{r}) \right],
$$

(8)

where the $P_l$ are the Legendre polynomials and their argument $\mathbf{k} \cdot \mathbf{R}$ is the cosine of the angle between $\mathbf{k}$ and $\mathbf{R}$. The impurity is taken to be centered at the origin. $R_l(\mathbf{r})$ is a radial solution of the Schrödinger equation and $j_l$ is a spherical Bessel function. If we take the potential to be of muffin-tin form, the exterior solutions can be expressed in terms of the phase shifts $\delta_l$ as follows\textsuperscript{24}:

$$
R_l(\mathbf{r}) = e^{i \delta_l} [ j_l(\mathbf{k} \mathbf{r}) \cos \delta_l - n_l(\mathbf{k} \mathbf{r}) \sin \delta_l ],
$$

(9)

where $n_l$ represents a spherical Neumann function. Expression (9) is valid for $\mathbf{r} > \mathbf{r}_{MT}$, where $\mathbf{r}_{MT}$ is the muffin-tin radius. It is apparent from Eqs. (1) and (2) that we are interested in the case $\mathbf{k} = k_F$, and thus the $\delta_l$ are the phase shifts at the Fermi energy.

We now restrict our attention to impurities which scatter electrons isotropically, i.e., $s$-wave scatterers. (An example of such an impurity is hydrogen in copper.\textsuperscript{29}) Since now only the $l = 0$ phase shift is appreciable, the sum over $l$ in Eq. (8) contains only the $l = 0$ term. The wave function in the exterior region ($\mathbf{r} > \mathbf{r}_{MT}$) then becomes

$$
\psi(\mathbf{F}) = \frac{1}{\Omega_1^{1/2}} \left[ e^{i \mathbf{F} \cdot \mathbf{R}} + \delta(\mathbf{r}) \right],
$$

(10)

where the scattered wave $\delta(\mathbf{r})$ is given by

$$
\delta(\mathbf{r}) = j_0(\mathbf{k} \mathbf{r}) e^{i \delta} - n_0(\mathbf{k} \mathbf{r}) e^{i \delta},
$$

(11)

and $\delta$ denotes the $l = 0$ phase shift.

We can now evaluate $n_0(\mathbf{F})$ using expressions (1), (2), (10), and (11). The result is

$$
n_0(\mathbf{F}) = \frac{2k_F^2 e^2 \epsilon_0}{\pi^2} \left[ \Gamma_{BF}(\rho) + \Gamma_{RRD}(\rho) \right],
$$

(12)

where $\theta$ is the angle between $\mathbf{F}$ and $\mathbf{R}$. The functions $\Gamma_{BF}$ and $\Gamma_{RRD}$ will be seen to describe the Bosniewicz–Friedel (BF) dipole\textsuperscript{14} and the RRD, respectively. They are given by

$$
\Gamma_{BF}(\rho) = -\frac{1}{2\rho^3} \left( 1 - 2 \rho \right),
$$

(13)

and

$$
\Gamma_{RRD}(\rho) = -\frac{1}{2\rho^3} \left( 1 - 2 \rho \right),
$$

(14)

The argument $\rho$ is $k_F r$. The above expressions are valid for $\mathbf{r} > \mathbf{r}_{MT}$. Since we can, in principle, imagine $\mathbf{r}_{MT}$ to be of arbitrarily short range, $\rho$ can also be taken to be arbitrarily small. In the small-$\rho$ limit, $\Gamma_{BF} \to -\rho/3$ and $\Gamma_{RRD} \to -\rho/3$.

In the limit of weak scattering ($\delta \ll 1$), $\Gamma_{BF}$ is proportional to $\delta$ and hence proportional to the impurity potential strength. This is precisely the behavior of the dipolar distribution originally derived by Bosniewicz and Friedel.\textsuperscript{14} Thus $\Gamma_{BF}$ describes the BF dipole. $\Gamma_{RRD}$ on the other hand, is proportional to $\sin^2 \delta$, and hence to the cross section. This is characteristic of Landauer’s RRD.\textsuperscript{1} For large $\rho$ there is a nonoscillatory component of $\Gamma_{RRD}$, namely the $1/\rho^3$ term in expression (14). This leads to an asymptotic $n_0(\mathbf{F})$ which is consistent with a general asymptotic RRD expression derived by Schalch.\textsuperscript{5,11} Further discussion of the BF vs RRD separation is given at the close of Sec. IV.

Plots of $\Gamma_{RRD}(\rho)$ and $\Gamma_{BF}(\rho)$ are shown in Fig. 1. We note that there is no special behavior near the origin associated with $\Gamma_{RRD}$. For small $\rho$ the $1/\rho^3$ term which gave the asymptotic RRD behavior
in $\Gamma_{\text{RRD}}$ has been analytically absorbed by the Friedel oscillations of the other terms.\(^\text{26}\)

Having obtained an expression for $n_0(\bar{r})$, we can determine the true electron density $n(\bar{r})$ by means of the Fourier-transform expression (3). For simplicity we evaluate $n(\bar{r})$ in the regime that the Thomas-Fermi screening length is shorter than other relevant lengths in the problem. In principle, this can be a valid regime. In practice, however, the screening length is not much shorter than the electron wavelength. We return to this point in Sec. IV. The Thomas-Fermi dielectric function is particularly simple in the regime of small screening length: It reduces to $\varepsilon(q) = \alpha^2/q^2$, where $\alpha$ is the Thomas-Fermi wave vector. For a parabolic band of electrons, $\alpha$ equals $(4m^2e^2/\pi\hbar^2)^{1/3}$, showing that a small screening length $1/\alpha$ can always be arranged, in principle, by appropriate choice of $k_F$ and the effective mass $m$.

Using this $q \to 0$ form of the Thomas-Fermi dielectric function $\varepsilon(q)$, we deduce from Eq. (4) that

$$n(\bar{r}) = -\alpha^2 q^2 n_0(\bar{r}).$$

Upon evaluating $\nabla^2 n_0(\bar{r})$ with $n_0(\bar{r})$ given by Eq. (12), we find

$$n(\bar{r}) = -\frac{2E_e F_0}{\alpha^2 q^2} \left( \frac{\cos \delta}{r^3} \right) [G_{BF}(\rho) + G_{\text{RRD}}(\rho)],$$

where

$$G_{BF}(\rho) = \left[ -\frac{2}{\rho^3} + \frac{2}{\rho^2} - \frac{4}{\rho} \right] \cos 2\rho$$

$$+ \left( \frac{4}{\rho^2} - 2 \right) \sin 2\rho \sin \delta \cos \delta$$

and

$$G_{\text{RRD}}(\rho) = \left[ \left( \frac{4}{\rho^2} - 2 \right) \cos 2\rho + \left( \frac{4}{\rho} - \frac{2}{\rho^3} \right) \sin 2\rho \right] \sin^2 \delta$$

(18)

correspond to BF and RRD contributions, respectively. The results are plotted in Fig. 2. Note that for small $\rho$, $G_{BF}/r^2 \to 0$ while $G_{\text{RRD}} - \frac{1}{\sin \delta}$.

Of vital importance in discussions of the RRD, especially as it applies to electromigration,\(^8\) is the spatial extension of the RRD. To obtain this we calculated the dipole moment of the true electron distribution associated with the RRD. The dipole moment $\mu$ of all charge contained within a radius $r$ is given by

$$\mu(r) = -e \int u(r - r')n(\bar{r}')z'd\bar{r}'$$

(19)

where $u$ is the step function defined by $u(x) = 1$ for $x > 0$ and $u(x) = 0$ for $x < 0$. The dipole moment is along the $z$ direction, which is the direction of $\vec{E}_0$.

The RRD dipole moment contains only the $G_{\text{RRD}}$ contribution to $n(\bar{r}')$ in Eq. (19). The result for the RRD dipole moment is

$$\mu(r) = \mu_0 \left[ \frac{1}{3} + \frac{2}{3} \cos 2\rho - \frac{1}{3} \left( \frac{2}{\rho} - \rho \right) \sin 2\rho \right],$$

(20)

where

$$\mu_0 = -\frac{2meF_0}{k_F} \sin^2 \delta$$

(21)

would be the value of the dipole moment for the RRD given by Landauer if $s$-wave scattering is assumed in Landauer's expression.\(^1\) The quantity $\mu(r)$ is plotted in Fig. 3. We note that for $r \to \infty$,

FIG. 2. Quantities $G_{\text{RRD}}$ and $G_{BF}$ vs $\rho$. These quantities are related to the screened density $n(\bar{r})$ by Eq. (16). As in Fig. 1, the values displayed do not include the $\sin^2 \delta$ and $\sin \delta \cos \delta$ factors for the RRD and BF quantities, respectively.
our $\rho(\tau)$ diverges as $\tau \sin 2k_{\rho}\rho$. The conclusion is that there is no localized dipole moment associated with the RRD distribution.

We now calculate the local field $\delta \overline{E}$ according to Eq. (7). The electrical potential $\phi$ to be used in that equation is the Thomas-Fermi potential $\phi(\overline{T}) = -\frac{1}{\rho} \exp(-\alpha \rho)$. It is convenient to integrate Eq. (7) by parts and obtain for the local field the result

$$\delta \overline{E}(\overline{T}) = - \int \phi(\overline{T} - \overline{R}) \frac{\partial n_0(\overline{T})}{\partial \overline{T}} d^3\tau.$$  \hspace{1cm} (22)

Again, for simplicity, we assume that the screening length $1/\alpha$ is much smaller than the scale of variation of $n_0(\tau)$. Equation (22) immediately reduces to

$$\delta \overline{E}(\overline{T}) = 4\pi e \frac{\partial n_0}{\partial \overline{T}} |_{\tau = \overline{T}}.$$  \hspace{1cm} (23)

Equation (23) implies that the local electrical potential is proportional to $n_0$. The local potential $\phi$ at any position is related to the local field at that position according to the defining equation

$$\delta \overline{E}(\overline{T}) = -\nabla \phi(\overline{T}),$$  \hspace{1cm} (24)

where $\nabla = \partial / \partial \overline{T}$ and where we have now used the variable $\overline{T}$ rather than $\overline{R}$ to denote a general point in space where the fields are to be calculated. It follows from Eqs. (23) and (24) that

$$\phi(\overline{T}) = -4\pi e \alpha^2 \delta n_0(\overline{T}).$$  \hspace{1cm} (25)

Thus, the quantities $\Gamma_{\text{BF}}$ and $\Gamma_{\text{RRD}}$ appearing in Eqs. (12)–(14) and displayed in Fig. 1 are actually the BF and RRD components of the local potential field. For $\tau \to \infty$ the average field is clearly dominated by the term $4\rho^2\sin^2\theta$ in $\Gamma_{\text{RRD}}$ since the term involving $\cos 2\rho$ averages to near zero over a volume containing several electron wavelengths.

When the leading asymptotic term in $\Gamma_{\text{RRD}}$ is used in Eq. (25), it is easily seen that the resulting potential field is precisely the electrostatic field arising from a dipole whose value is $p_0 \hat{z}$, where $p_0$ is defined by Eq. (21) and $\hat{z}$ is a unit vector in the direction of $\overline{E}_0$. This verifies Landauer's picture for the long-range average field of the RRD.

It is of interest to have an explicit expression for the electric field $\delta \overline{E}$. The component of the local field in the $z$ direction is easily obtained from Eqs. (24) and (25) and the $n_0(\overline{T})$ expression (12). We find

$$\delta \overline{E}_z = \frac{8\pi k^2 T E_0}{\tau_{\overline{T}}^2} \left[ \frac{\Gamma(\rho)}{\rho} \sin^2 \theta + \frac{d\Gamma(\rho)}{d\rho} \cos^2 \theta \right],$$  \hspace{1cm} (26)

where in Eq. (26) the RRD field is obtained by inserting $\Gamma_{\text{RRD}}$ for $\Gamma$, while the BF field is obtained by inserting $\Gamma_{\text{BF}}$ for $\Gamma$. The results for $\Gamma/\rho$ and $d\Gamma/\rho$ are plotted in Fig. 4. The BF field is regular for $\tau \to 0$. There is an apparent divergence in $\Gamma_{\text{RRD}}(\rho)/\rho$ since $\Gamma_{\text{RRD}}(0)$ does not vanish. However, recall that our expressions apply for $\rho \gg \rho_{\text{MT}}$ only. Inside the muffin tin the interior solutions $E_{\pm}(\rho)$ are well behaved and $\delta \overline{E}_z$ is, of course, finite.
IV. DISCUSSION

We have evaluated the microscopic field and charge density around an s-like impurity scatterer in a jellium background. The field given by Eq. (26) gives precisely the asymptotic behavior obtained by Landauer in a semiclassical analysis.\(^1\) A superposition of such dipole fields gives the extra field needed to drive electrons past a region containing impurities.

If one considers a conductor in which the only source of scattering is impurity scattering, then one is led to the conclusion that there is, in fact, no true external field. Rather, there is only a self-consistent field internally generated by a superposition of RRD's. It is this superposition which yields the macroscopic electric field in a metal. To a certain extent, then, "exact" quantum-mechanical derivations of transport phenomena are less than rigorous since in such treatments an external field is taken as the perturbation in the system Hamiltonian. (This, of course, was also assumed here since the expressions used in Sec. II were based on the "exact" Kubo formalism.)

As we have discussed elsewhere,\(^4\) there are standard tricks to short-circuit the internally generated RRD field. Among these tricks are the assumption of toroidal geometry, periodic boundary conditions, or an "infinite medium," i.e., a medium where average dipole fields are taken to vanish by "symmetry." None of these methods is free of objections.\(^4,7\) Nonetheless, the procedure used here and outlined elsewhere\(^4\) is sensible. First we focus on a small region (within a mean free path) around the impurity. Everything outside this region is treated as setting up an external field within the region. This enables us to obtain a local field using Kubo theory. Finally, we find that our local field summed over all impurities is precisely the field assumed in the first place. This closes the self-consistency loop. Although this procedure gives no new results for the conductivity in a homogeneous medium, it does imply that great care is needed in treating inhomogeneous media when the scale of the inhomogeneity is comparable to a mean free path.

Perhaps the most surprising feature of our calculation is the elusive nature of the RRD charge distribution. It is not localized within the order of screening lengths or electron wavelengths. Instead, the RRD is hidden, chameleonlike, within the Friedel oscillations which extend to large distances around the impurity. At large distances it appears as though the average RRD field is emanating from a dipole at the origin. If one were to ignore all oscillatory terms involving \(\cos 2\rho\) and \(\sin 2\rho\) in Eqs. (13) and (14), then it would also appear as if the RRD were a dipole of strength \(\rho_0\) at the origin. But this is misleading since there is no RRD singularity at the origin; the oscillatory terms combine with the would-be singular term to give smooth behavior with no localized dipole near the impurity. This is seen in the figures.

We note from expression (26) and Fig. 3 that the field of the RRD near the impurity is opposite to the external field. Also, the true charge density \(-en(\overline{\mathbf{F}})\) due to the RRD near the impurity is in the opposite sense to that expected for a localized dipole moment \(\rho_0\) near the impurity. The BF field near the impurity is opposite to \(\mathbf{E}_0\) for an attractive potential \((\delta > 0)\) and in the direction of \(\mathbf{E}_0\) for a repulsive potential \((\delta < 0)\). The BF force on the impurity is thus always in the direction of the electron wind. It is clear from the figures that the structure in the RRD and BF fields cannot simply be attributed to localized dipoles. The Friedel oscillations are an essential part of the near- and far-field structure.

We now discuss implications for the driving force in electromigration. Our results apply to the calculation of the force exerted on a weak, very localized scatterer due to the presence of a strong s-like scatterer in its vicinity. This force corresponds to an interference effect between two scatterers and has thus far been calculated only from weak-scattering expressions.\(^16,17\)

The force on the weak scatterer can be simply obtained from Eq. (6) by first integrating by parts. The result, analogous to Eq. (22), is

\[
F_z = -\int V(\overline{\mathbf{F}} - \overline{\mathbf{R}}) \frac{\delta n(\overline{\mathbf{F}})}{\delta z} d^3r, \tag{27}
\]

where \(V\) is the (screened) potential of the weak scatterer. We now assume a very localized scatterer modeled by a delta-function potential \(V = A\delta(\overline{\mathbf{F}} - \overline{\mathbf{R}})\), where \(A\) is the strength parameter. With this form Eq. (27) becomes

\[
F_z = - \frac{A\alpha^2}{4\pi\varepsilon} \delta E_z, \tag{28}
\]

where \(\delta E_z\) is the local field at the position of the weak scatterer and is given by Eqs. (23) or (26). Equation (28) gives the force on the weak scatterer correct to linear order in the strength of the weak scatterer. The discussion we have given for \(\delta E_z\) (see Fig. 3) thus applies to the force \(F_z\).

We comment on the apparent large RRD contribution to the force \(F_z\) and the field \(\delta E_z\) as \(r \to 0\). This behavior arises from the \(1/\rho\) divergence in the term \(\mathbf{f}_{\text{RRD}}/\rho\) in Eq. (26). The divergence appears in the RRD term and not the BF term because in the exterior solution given by Eq. (11)
the “singular” $n_{i=0}$ term contributes to $\Gamma_{RBD}$, while the “well behaved” $j_{i=0}$ term contributes to $\Gamma_{BF}$.

If we wish to claim that $\gamma = 0$ is a physically relevant domain for our expressions, we must also choose $r_{MT} = 0$ since we have used solutions valid for $r > r_{MT}$ only. The condition $r_{MT} = 0$ and the condition that only $s$-wave scattering is appreciable places severe restrictions on the impurity potential and the resulting value of $\delta$. For example, to satisfy these conditions for a spherical-well model potential we need a very deep potential and small $\delta$. As a result of small $\delta$, the BF contribution would dominate the force on an isolated impurity. In fact, it is generally true that the force on an isolated impurity is in the direction of the electron wind, i.e., in the direction of the BF force. This has been established from $T$-matrix expressions\textsuperscript{6,7} which are rigorous consequences of the expressions (1) and (6) used here.

We emphasize that a weak scattering treatment of the $s$-wave scatterer would give a spatial variation of the field exactly like the BF field which we have calculated. The lowest-order perturbation-theory result simply replaces the $\sin \delta \cos \delta$ factor in $\Gamma_{BF}$ by the factor $\delta$. The RRD fields do not, however, appear in lowest-order perturbation theory. Therefore, to the extent that the RRD fields are comparable to, or exceed, the BF fields in Fig. 4, one must go beyond perturbation theory and use the strong-scattering theory presented here. Typically $k \cdot r_{MT} \sim 1$ for metals, so that $\rho > 1$ is the appropriate region in the figures. In that region the BF and RRD terms are comparable, except that $\Gamma_{BF}$ contains the factor $\cos \delta \sin \delta$ while $\Gamma_{RBD}$ contains the factor $\sin ^2 \delta$.

As an example, if $\delta \sim 0.3$, the RRD fields are around 30% of the BF fields. The most dramatic differences show up at resonance ($\delta = \pi/2)$, where the BF contribution vanishes entirely. Furthermore, the structure of the RRD fields and BF are always different. It is not possible to simulate RRD contributions simply by changing $\delta$ or choosing a “better” potential or pseudopotential.

The distinction between the RRD and BF contributions to the force $F_\delta$ also arises in $T$-matrix expressions. A $T$-matrix expression which is equivalent to Eq. (27) is\textsuperscript{6}

$$ F_\delta = \frac{2\pi i}{\hbar} \sum_{k, k'} \frac{\partial}{\partial R_z} \left( \langle \bar{k} | T^{\alpha} | k \rangle \langle \bar{k'} | T^{\alpha*} | k' \rangle \delta (\epsilon_{\bar{k}} - \epsilon_{\bar{k'}}) \right), $$

(29)

where $R_z$ is the $z$ coordinate of the impurity on which the force is to be calculated and $T^{\alpha}$ and $T^{\alpha*}$ denote the $T$ matrix for the localized impurity complex. (The $\pm$ signs denote electron or hole propagators in the defining equation for $T$.)

If Eq. (29) is applied to the problem of a strong $s$-wave scatterer and a weak second scatterer, expression (28) is obtained to lowest order in $\tilde{\nu}$. If one approximates the $T$ matrix in a single-site picture, one writes $T^{\alpha} = t^{\alpha} + \tilde{\nu}$, where $t^{\alpha}$ represents the $T$ matrix of the isolated strong scatterer. Using this in Eq. (29) and taking the real part of that expression, we find that $F_\delta$ is precisely the result we have obtained for the BF contribution alone. The RRD field is completely lost in this procedure. The RRD contribution requires one to include multiple scattering terms in $T^{\alpha}$ when evaluating Eq. (29), i.e., terms to all orders in the strong scatterer and first order in $\tilde{\nu}$. We have already seen that such terms are important, especially at resonance. We expect that these RRD-related terms would be important corrections in single-site calculations of cluster scattering forces and resistivities for clusters of strong scatterers in both solid and liquid metals.\textsuperscript{17,27}

We comment on our approximations. The central approximation is the use of linear screening. As far as we are aware, this approximation is common to all previous self-consistent treatments of fields and charges in electron transport. A discussion of linear versus non-linear screening has been given elsewhere\textsuperscript{28} in the context of Kubo formalism. An improved treatment of screening is not expected to lead to substantial changes in any of our results.

The particular assumption of short screening length simplifies the calculations and allowed us to obtain analytic expressions for fields and charge densities. Expressions which are valid independent of any screening-length assumptions include Eq. (12) for $n_e(\bar{F})$ and Eq. (28) for the force on a weak very localized scatterer. In using Eq. (28) for the force, one must use the $\delta E_\delta$ expression (26) even though this expression does not give the actual local field if the screening length is not small.

When the screening length is not small ($\alpha \approx k_F$), the Friedel oscillations we have found in $n(\bar{F})$ and $\delta E(\bar{F})$ will be somewhat washed out. In general, one would have to average our calculated $n(\bar{F})$ or $\delta E(\bar{F})$ over the region containing the Thomas-Fermi screening potential. For example, the true local field would be given by

$$ \delta E_\delta (\bar{F}) = \frac{\alpha^2}{4\pi} \int \frac{e^{-\alpha |\bar{r} - \bar{r}'|}}{|\bar{F} - \bar{F}'|} \delta E_\delta (\bar{F}') d^3r', $$

(30)

where $\delta E_\delta$ represents the calculated value for $\alpha \rightarrow \infty$, i.e., expression (28). The relation (30) also holds between the true density $n(\bar{F})$ and the calculated density $n_e(\bar{F})$, where $n_e(\bar{F})$ is given by
V. CONCLUSIONS

The RRD has been found to play an important role in the local field and electromigration driving forces. Our calculations give the first quantitative description of the RRD. The long-range (average) RRD field is exactly as described by Landauer. We found that the RRD does not arise from a very localized charge distribution around the impurity; rather, the RRD is extended and contains important contributions from long-range Friedel oscillations. Since our expressions are valid for distances up to a mean free path from the impurity, we conclude that the sources of the RRD are effectively distributed over a distance on the order of a mean free path from the impurity.

The RRD contributions to the electromigration driving force has been calculated for the case of a weak scatterer near a strong scatterer [Eq. (28)]. This RRD contribution is missing in previous calculations based on perturbation theory or singlesite $T$ matrices. RRD corrections are appreciable, and near a scattering resonance they become dominant.

Finally, we comment on the separation of RRD and BF terms throughout our analysis. The total charge density (BF + RRD) is, of course, the relevant physical quantity. The fact that the charge density neatly separates into parts which we define as BF and RRD quantities is convenient, but not essential, in our investigation. The BF and RRD densities are precisely defined in Eqs. (13) and (14) according to whether they exhibit $\sin^2\delta$ behavior (RRD) or $\sin\delta\cos\delta$ behavior (BF). The RRD quantities are thus proportional to the cross section as in Landauer’s treatment. The BF quantities are identical to the perturbation-theory results of Bosvieux and Friedel when one invokes the weak-scattering limit $(\delta \ll 1)$ and replaces $\sin\delta\cos\delta$ by $\delta$ in our expressions. Note that the RRD distribution does contain some “interference” terms and Friedel oscillations as well as the $\gamma^{-2}$ asymptotic behavior, and is thus not precisely the quantity which has been envisioned by Landauer. The separation of the interference terms and the Friedel oscillations from the RRD distribution is only possible in the asymptotic limit. However, such asymptotic separations have no meaning close to the impurity, i.e., there is no meaningful analytic continuation of the asymptotic form to the $\gamma \to 0$ limit. Our calculations show that there is no localized dipolar charge near the impurity on a microscopic scale. However, on the macroscopic scale there are electric fields set up which appear to emanate from a microscopically localized dipolar charge. These are our main conclusions and they are not dependent on the fact that we have made a particular separation between BF and RRD quantities.

We emphasize this point because the BF and RRD separation is not so neatly made when the scattering potential is more complicated, for example, when several phase shifts are appreciable. One could, in that case, still follow the general analysis of this paper, but without explicitly separating the charge density into RRD and BF quantities.

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11An expression for the RRD electronic density far from the impurity is reported by Schachl in Ref. 6. Schachl has actually calculated the asymptotic form of the unscreened RRD density, i.e., the $\gamma \to \infty$ limit for the quantity $n_{\gamma}(\Phi)$ defined by our Eq. (1).
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calculations were only performed linear in $V$. In addi-
tion, an unphysical result is obtained, namely, the
force on an impurity in an external field $E_0$ is found to
be independent of the relaxation time $\tau$ for background
scattering. The force should have contained a term propor-
tional to $\tau E_0$, corresponding to the so-called
"wind force" in electromagnetism theories (see Refs.
4-8, 10, 12).
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sumed in Ref. 4 for the collision term in the Liouville
equation. The collision term is generally approximated
by $-\nabla p/\tau$, where $p$ is the density matrix and $\hat{n}$
is the density matrix to which $p$ relaxes. In Ref. 4 $\hat{n}$
was taken to be the equilibrium density matrix in the
absence of the field. In Ref. 19 Schaich uses a form
for $\hat{n}$ which leads to a solution for $p$, which conserves
particles at every point in space, i.e., the particle
trajectories remain continuous even in the presence of
collisions with the background. Since local conserva-
tion of particles describes physically correct behavior,
Schaich’s form for $\hat{n}$ is preferable to the form used in
Ref. 4. However, for large $k\ell$ (or large $\epsilon_0\tau$) both
choices for $\hat{n}$ give virtually identical fields and forces.
The point is that the leading contribution to $p$ turns
out to be proportional to $\tau$ and hence the collision
term is of zero order in $\tau$. Since there are other
terms in the Liouville equation (for the off-diagonal
elements of $\rho$) which are linear in $\tau$, they completely
dominate the collision term for $\tau \to \infty$. The form as-
sumed for $\hat{n}$ is thus unimportant in the regime of physi-
ical interest, i.e., for $k\ell \gg 1$. (A similar conclusion
holds for the collision term in the semiclassical anal-
ysis, e.g., the Boltzmann-equation analysis of Ref.
13.) Note, however, that imposition of the $\tau \to \infty$ limit
and the consequent ignoring of the collision term ef-
ectively excludes us from addressing the problem of
the electrostatic screening of the direct field; the
latter is formally of order $1/k\ell$ times the dynamic
screening considered here (see Ref. 20).
22This result can be derived from Sham’s analysis (Ref.
7) by considering his response functions with the force
vertex replaced by the electron-density vertex. The
insertion of random-phase approximation bubble dia-
grams just before this vertex has the effect of replacing
the unscreened density response $n(\ell)$ by the screened
density response $n(\ell)/\epsilon(\ell)$. An explicit derivation of
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(i.e., s-wave scatterers), all contributions $n_0|\psi(\ell)|^2$
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