PHYSICAL REVIEW B VOLUME 16, NUMBER 12 15 DECEMBER 1977

# Local fields in electron transport: Application to electromigration*

R. S. Sorbello and Basab Dasgupta

*Department of Physics, University of Wisconsin-Milwaukee, Milwaukee, Wisconsin 53201*

(Received 6 July 1977)

A quantum-mechanical expression is given for the local electric field in dc electron transport. The local field is shown to provide the driving force for the migration of atoms during dc electron transport (electromigration). We express the local field in terms of the electron charge density, which we obtain by solving the Liouville equation for the single-particle density matrix. The solutions are found within a self-consistent field weak-scattering approximation scheme for an impurity in a jellium background. Electron-phonon interaction is included via a phenomenological relaxation time. It is shown that the local field arises from both static and dynamic screening. The static screening is associated with the screening of the external field near the impurity, while the dynamic screening is associated with the "electron-wind force," or the momentum transferred by the electrons in collisions with the impurity. It is found that the "electron-wind force" dominates when $k_F l \gg 1$, where $k_F$ is the Fermi wave vector and $l$ is the electron mean free path. Only when $k_F l$ is of order unity are the static and dynamic screening contributions comparable. Landauer's residual-resistivity dipoles and carrier-density-modulation effect are investigated, and are found to contribute to the local field. The carrier-density modulation effect is shown to lead to deviations from Matthiessen's rule by shifting the Fermi energy relative to the band bottom. Within the local-field framework, we discuss the distinction between the external field and long-range macroscopic fields in quantum-mechanical formulations of dc electron transport.

## I. INTRODUCTION

In discussing dc electron transport near inhomogeneities it may be convenient to introduce the concept of the local electric field. The local-field concept turns out to be especially useful in describing the migration of impurities and other defects during electron transport. In fact, the local field is the driving force for the migration of atoms in the presence of the external electric field and the accompanying electron current. This migration phenomenon is known as electromigration. The local electric field is also a relevant driving force in thermomigration, or atomic migration in a temperature gradient. Theories of electromigration and thermomigration have been reviewed in the recent literature.[1-5]

The local electric field arises from all electrical charges in the system, including the sources of the external field. Part of the electrical charge distribution may be associated with the electron current flow, and corresponds to the "electron wind" or dynamic screening in electromigration theories. An additional contribution may be associated with static screening of the external field. The statically screened external field gives rise to the "direct-field" force in electromigration theories. The magnitude of the "direct-field" force has been controversial. For example, according to some theories[6-8] the "direct-field" force vanishes (complete static screening) in the vicinity of an interstitial impurity, while in other theories[9-16] there is no static screening.

To settle these controversies it is necessary to determine the local electric field by solving the quantum-mechanical transport problem for the response of electrons in an external dc electric field. Several powerful techniques have been introduced for treating the electron-transport problem.[17-22] It has been found that for sufficiently long electronic mean free paths, the electrical conductivity calculated quantum mechanically reduces to the electrical conductivity obtained from the Boltzman equation.[22] This reduction has been possible only in the weak-scattering or dilute-scattering limit. When interference effects between scatterers are allowed, extra contributions to the transport equation emerge.[17] Additional corrections to the Boltzmann equation might also arise from current-flow inhomogeneities,[23] or possibly from Landauer's residual-resistivity dipoles,[24,25] and his carrier-density modulation effect.[24,26]

Further difficulties in the Boltzmann-equation approach arise when quantities such as charge density and local fields are to be determined. The problem is that such quantities involve off-diagonal elements of the density matrix in the Bloch representation, whereas strictly speaking the Boltzmann equation is only relevant for the diagonal elements.[17] While it may be legitimate to ignore this difficulty within a fully semiclassical problem in which the scattering potentials are slowly varying in space, this semiclassical picture is highly suspect for the case of highly localized scatterers such as atomic defects. For this reason, charge densities and local fields which are derived from the use of the Boltzmann equation may be of very limited validity.

To avoid the difficulties inherent in semiclassical pictures, we base our calculation on the quantum-mechanical Liouville equation for the density matrix. Our calculation is an application of the method introduced by Kohn and Luttinger[17] (KL). One advantage of this method is that we shall be able to extend into the quantum-mechanical regime the very physical semiclassical analysis of Das and Peierls.[16] This will lead to a better physical understanding of the various sources of the local electric field. In particular, we shall be able to isolate the contributions due to the "direct field" and the "electron wind," as well as investigate the effects of the residual-resistivity dipoles and carrier-density modulation.[23-26]

The present calculations, like those of Das and Peierls,[16] will be confined to the model of dilute weakly scattering impurities in jellium, with phonon scattering introduced via a phenomenological relaxation time. The results we shall obtain are consistent with recent results obtained within the framework of linear-response theory.[13-15]

## II. LOCAL ELECTRIC FIELD

In analogy with classical electrostatics we can define the local microscopic electric field at some position $\vec{X}$ by introducing a point test charge of magnitude $Q$ at $\vec{X}$. If the force exerted on the test charge is denoted by $\vec{F}_Q(\vec{X})$, we define the local electric field $\vec{E}_L(\vec{X})$ by the expression

$$\vec{E}_L(\vec{X}) = \lim_{Q\to 0} \vec{F}_Q(\vec{X})/Q . \tag{1}$$

The mass $M$ of the test particle is assumed to be very large (formally $M \to \infty$) so that in calculating the force we can ignore the motion of the test particle. We then visualize the test particle as a sharply localized wavepacket, which represents a classical particle essentially fixed at position $\vec{X}$.

In order to obtain $\vec{F}_Q(\vec{X})$ we apply the results given elsewhere for the force on an ion.[13] The force on any ion of valence $Z$ at position $\vec{X}$ in the presence of an external field $\vec{E}$ is given by[13]

$$\vec{F} = Ze\vec{E} - \int n(\vec{x})\, \frac{\partial V_0(\vec{X}-\vec{x})}{\partial \vec{X}}\, d^3x . \tag{2}$$

Here $e$ is the charge of the proton, $n(\vec{x})$ is the exact quantum-mechanical electron density at position $\vec{x}$, and $V_0(\vec{X}-\vec{x})$ is the bare interaction energy between an electron at $\vec{x}$ and the ion in question. The integral is over all space. Since we are interested only in that part of the force $\vec{F}$ which depends on $\vec{E}$, we need only retain in $n(\vec{x})$ that part of the density which depends on $\vec{E}$. In Eq. (2) and henceforth we take $n(\vec{x})$ to be the $\vec{E}$-dependent electron density in the absence of the test charge.

In deriving Eq. (2) one assumes that the ions are rigid and essentially fixed in position. The core electrons are not treated dynamically; their polarization in the external field is ignored.

It is clear from the derivation[13] of Eq. (2) that this equation is valid for any external field of arbitrary space and time dependence, i.e., we can take $\vec{E} = \vec{E}(\vec{X}, t)$. In this case $n(\vec{x})$ will of course be time dependent due to the coupling of the electrons with the external field. In the present dc transport problem we take $\vec{E}$ to be constant in space and time.

Result (2) is a generalization of the Feynman-Hellman theorem[27] to a nonequilibrium, dissipative system. In the usual derivation of that theorem one starts with the expression $\vec{F} = -\partial\langle\mathcal{H}\rangle/\partial\vec{X}$, where $\langle\mathcal{H}\rangle$ is the expectation value of the total system Hamiltonian $\mathcal{H}$. Such an expression is not valid for open, dissipative systems such as that considered in electron transport. The correct starting point for dissipative systems is the equation of motion of the expectation value of the momentum of the ion. The ion is taken to be moving infinitely slowly as a sharply localized wavepacket whose dynamics are governed by $\mathcal{H}$. This is the approach used to derive Eq. (2).[13]

We now apply Eq. (2) to the particular case of the force on the test particle of charge $Q$. The interaction between the test charge and an electron is $V_0(\vec{X}-\vec{x}) = -Qe/|\vec{X}-\vec{x}|$. Using Eqs. (1) and (2) we obtain

$$\vec{E}_L(\vec{X}) = \vec{E} - \int n(\vec{x})\, \frac{\partial}{\partial \vec{X}}\, \frac{-e}{|\vec{X}-\vec{x}|}\, d^3x \tag{3}$$

where the $Q\to 0$ limit has brought in $n(\vec{x})$, the electron density in the absence of the test particle but in the presence of all the ions in the system.

Since $n(\vec{x})$ is independent of $\vec{X}$ we can recast Eq. (3) in the suggestive form

$$E_L(\vec{X}) = \vec{E} - \frac{\partial \Phi(\vec{X})}{\partial \vec{X}} , \tag{4}$$

where $\Phi(\vec{X})$ is the local electrostatic potential defined by

$$\Phi(\vec{X}) = -e \int n(\vec{x})\, \frac{1}{|\vec{X}-\vec{x}|}\, d^3x . \tag{5}$$

It should be emphasized that despite the classical form of Eqs. (2)–(5), these equations include the electronic many-body effects. The latter are contained within $n(\vec{x})$.

It is interesting that Eqs. (4) and (5) imply that one could have obtained the correct force on the test particle by simply computing the change in the expectation value of the interaction energy as the particle is moved. That is, one can write

$$\vec{F}_Q(\vec{X}) = -\frac{\partial\langle V'\rangle}{\partial\vec{X}}, \tag{6}$$

where $V' = -Q\vec{X}\cdot\vec{E} - \sum_l Qe/|\vec{X}-\vec{x}^{(l)}|$ and the sum is over all electrons, with the position of the $l$th electron denoted by $\vec{x}^{(l)}$. Equation (6) is valid only for the force on the test particle to order $Q$. One cannot apply Eq. (6) to the force on an ion by simply changing $Q$ to $Ze$ in the expression for $V'$. The resulting expression would agree with the correct expression (2) only to terms linear in $Z$ in the $Z \to 0$ limit.

The connection between the force on an ion and the local field follows immediately by comparing Eqs. (2) and (3). For a point-ion potential the force expression (2) gives $\vec{F} = Ze\vec{E}_L$. In the more general case of an ion core of finite size, we can write

$$\vec{F} = \int N(\vec{X})\vec{E}_L(\vec{X})\,d^3X, \tag{7}$$

where $N(\vec{X})$ is the charge density of the bare ion (nucleus plus core electrons). $N(\vec{X})$ and $V_0$ are related by the Poisson equation $\nabla^2 V_0(\vec{X}) = 4\pi e N(\vec{X})$.

It should be emphasized that by assuming all ions to be rigid we are explicitly ignoring the dynamics of the core electrons in the external field. If we wish not to invoke this rigid-ion picture, then Eqs. (3) and (7) will remain valid provided that in Eq. (3), $n(\vec{x})$ includes the correct core-electron density in the presence of $\vec{E}$, and in Eq. (7), $N(\vec{X})$ is the nuclear charge only.

Now, for core levels well separated from the conduction band, the core electrons are expected to polarize essentially as in a free ion. This implies that for an ion of valence $Z$, the core polarization cancels the effect of the field on all but $Z$ protons in the nucleus. The core polarization is a very slight dipolar deformation in the core-electron wave functions.[28] This polarization produces a field near the nucleus which is comparable to the external field $\vec{E}$.[29] However, in the important region outside the core this polarization field is not significant. There are two reasons for this: First, the dipolar sources of the core-polarization field are localized within the core,[28] and hence the field is substantially weakened at distances of two or three core radii from the nucleus. Second, the core-polarization field is screened out by the conduction electrons at distances greater than a screening length from the nucleus. Thus it appears to be a good approximation to use the rigid-ion approximation and ignore the dynamics of those core electrons coming from core levels well below the conduction band bottom. (Of course, core electrons that fall within the conduction band are to be treated dynamically and are not considered as part of the rigid ion.)

It is worth remarking that the electric field $\vec{E}$ appearing in our equations is to be regarded as an external uniform field whose sources are *not* to be screened. It would be incorrect to regard $\vec{E}$ as a longitudinal field arising from external charges imbedded in the medium since static electronic screening would prevent the field from penetrating very far into the metal. The imposition of the no-screening condition on $\vec{E}$ for dc transport is typically done in an *ad hoc* way,[30] or equivalently, a transverse field is used.[31] In either case an infinite medium (or periodic boundary conditions) is assumed.

Using the no-screening condition in an infinite medium is a device to enable one to avoid the complications of the physical boundary conditions in the dc transport problem. For example, we need not explicitly consider the self-consistent charges which are set up at an interface between two dissimilar metals, as at the electrode-metal interface at the ends of the sample. These charges are responsible for the electric field which drives the current through the sample, and arise not from imbedded external charges, but rather from the self-consistent electron-scattering process as envisioned by Landauer[25] (see Sec. IV C). In our model of an infinite medium there is no polarization-charge buildup at the ends of the sample. (These charges can be obtained macroscopically for a finite sample of course by solving the macroscopic boundary-value problem.) We emphasize that variations in the local field due to scatterers (microscopic or macroscopic inhomogeneities) within the system will be correctly obtained from Eq. (3) provided that these scatterers are included in the system Hamiltonian.

A further advantage of considering the model of an infinite medium is that if there are only randomly distributed microscopic scatterers in the medium the external field $\vec{E}$ is precisely the macroscopic electric field. This is easily seen by noting that the macroscopic field is the spatial average of the local field $\vec{E}_L$, and that by symmetry the spatial average of the integral in Eq. (3) vanishes for the inifinite medium.[32]

A more rigorous justification for considering $\vec{E}$ to be the macroscopic electric field and for considering an infinite medium can be deduced from KL.[17] They considered the solution of the transport problem in a finite toroidal geometry, with the electric field caused by an axial magnetic field increasing with time. They found that the solution was consistent with that obtained for an inifinite medium (periodic boundary conditions).[33]

Moreover, in the toroidal geometry it is clear from symmetry that no distribution $n(\vec{x})$ can contribute to an average field, or net voltage drop, in a closed path around the torus. Hence, the external field $\vec{E}$ equals the macroscopic field here.

In quantum-mechanical calculations for any physical system the safest course to follow is to avoid identifying $\vec{E}$ with the macroscopic field. Instead the latter is determined in terms of $\vec{E}$ at the end of the calculation by setting the macroscopic field equal to the spatial average of $\vec{E}_L$ in the medium, where $\vec{E}_L$ is given by Eq. (3). This procedure is valid for any system regardless of the boundary conditions assumed. As an example, consider the model of a single localized scatterer in jellium. In this case $\vec{E}$ will equal the macroscopic field because the integral in Eq. (3) gives a field which is not appreciable far from the impurity (Sec. III).

These remarks concerning the distinction in quantum-mechanical theories between the external field and the macroscopic field have been motivated by questions raised by Landauer.[34]

## III. DENSITY-MATRIX CALCULATION OF LOCAL FIELD

### A. Liouville equation in self-consistent-field approximation

We determine the electron density $n(\vec{x})$ using a single-particle density-matrix approach similar to that of KL.[17] The system we shall consider is that of a weakly scattering impurity in a jellium background. Electron-phonon scattering is included through a relaxation time. Electron-electron interaction is treated within a self-consistent screening approximation. Electron-phonon and electron-electron interactions were not considered in KL.

Following for the most part the KL notation, we express the total one-electron Hamiltonian $H_T$ as follows:

$$H_T = H_0 + H' + e\vec{x}\cdot\vec{E}\,, \tag{8}$$

where $H_0$ is the kinetic energy of an electron and $H'$ is the electron-impurity interaction. $\vec{x}$ is the electron coordinate.

We are interested in the total one-electron density matrix, which we denote by $\rho_T$. This quantity is separated into a term $\rho$, which is the equilibrium density matrix (in the absence of $\vec{E}$, but in the presence of $H'$), and a term $f$ which is linear in the field. Corrections which are second order or higher in $\vec{E}$ are considered negligible. We therefore write

$$\rho_T = \rho + f\,. \tag{9}$$

Similarly, it is convenient to separate the electron-impurity interaction $H'$ into an equilibrium and field-dependent part as follows:

$$H' = V^0 + V^1\,, \tag{10}$$

where $V^0$ is the screened electron-impurity potential in the absence of $\vec{E}$, and is to be treated as a known quantity. $V^1$ is the screening part which is linear in $\vec{E}$ and is to be determined self-consistently.

With the separation (10), the explicit form of $\rho$ at temperature $T$ can be expressed as

$$\rho = \{\exp[(H_0 + V^0 - \epsilon_F)/k_B T] + 1\}^{-1}\,, \tag{11}$$

where $\epsilon_F$ is the Fermi energy and $k_B$ is Boltzmann's constant. We use units where $\hbar = 1$.

The density matrix satisfies the Liouville equation

$$\frac{\partial \rho_T}{\partial t} = -i[H_T, \rho_T] - \frac{(\rho_T - \rho)}{\tau}\,, \tag{12}$$

where we have introduced a relaxation time $\tau$ to describe the decay to equilibrium by dissipative processes. These processes may be electron-phonon scattering, or in general, any background-scattering mechanism not included in the interaction $H'$ between the electron and the impurity.

In the steady state, $\partial\rho_T/\partial t = 0$ and Eq. (12) can be cast into the form

$$if/\tau = [e\vec{x}\cdot\vec{E}, \rho] + [V^0, f] + [V^1, \rho] + [H_0, f]\,. \tag{13}$$

In obtaining Eq. (13) we have used Eqs. (8), (9), and (10) in Eq. (12) and have systematically discarded terms which are higher order in $\vec{E}$.

It is most convenient to express Eq. (13) in the plane-wave representation since plane waves are eigenfunctions of $H_0$, that is, $H_0|\vec{k}\rangle = \epsilon_{\vec{k}}|\vec{k}\rangle$ where $|\vec{k}\rangle$ is a plane wave state and $\epsilon_{\vec{k}} = k^2/2m$ is the energy eigenvalue. In the plane-wave representation Eq. (13) leads immediately to

$$f_{\vec{k}\vec{k}'} = \frac{[\rho, e\vec{x}\cdot\vec{E}]_{\vec{k}\vec{k}'}}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}'} - i/\tau} + \sum_{\vec{k}''} \frac{f_{\vec{k}\vec{k}''} V^0_{\vec{k}''\vec{k}'} - V^0_{\vec{k}\vec{k}''} f_{\vec{k}''\vec{k}'}}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}'} - i/\tau} + \sum_{\vec{k}''} \frac{\rho_{\vec{k}\vec{k}''} V^1_{\vec{k}''\vec{k}'} - V^1_{\vec{k}\vec{k}''} \rho_{\vec{k}''\vec{k}'}}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}'} - i/\tau}\,. \tag{14}$$

The unknown quantity $V^1$ appearing in Eq. (14) is determined self-consistently from the Poisson equation

$$\nabla^2 V^1 = -4\pi e^2 n(\vec{x})\,, \tag{15}$$

where the electron density $n(\vec{x})$ refers to that part of the total electron density which depends linearly on $\vec{E}$. The self-consistency cycle is closed by requiring that $n(\vec{x})$ arises directly from the quantum-mechanical wave functions, or equivalently, from the density matrix. This condition is conveniently expressed as

$$n(\vec{q})=\sum_{\vec{k}} f_{\vec{k},\vec{k}-\vec{q}}\,, \tag{16}$$

where $n(\vec{q})$ is the Fourier transform of $n(\vec{x})$, that is,

$$n(\vec{x})=\sum_{\vec{q}} n(\vec{q})\exp(i\vec{q}\cdot\vec{x})\,. \tag{17}$$

In Eqs. (16) and (17) the sums are over all $\vec{k}$ and $\vec{q}$, respectively. For convenience we have chosen a normalization which takes the crystal volume to be unity. The transformation from sum to integral is accomplished via the rule $\sum_{\vec{q}}\rightarrow(1/8\pi^3)\int d^3q$, with an additional factor of 2 needed for $\sum_k$ due to spin degeneracy.

It is convenient to rewrite the Poisson equation (15) in terms of Fourier-transformed quantities. Consistent with Eq. (17), we define the transform

$$V^1(\vec{q})=\int V^1(\vec{x})\exp(-i\vec{q}\cdot\vec{x})\,d^3x\,,$$

where the integration is over all coordinate space. We can then cast Eq. (15) into the Fourier-transformed form

$$V^1(\vec{q})=4\pi e^2 n(\vec{q})/q^2\,. \tag{18}$$

The quantity $V^1(\vec{q})$ is identical to the matrix element $V^1_{\vec{k},\vec{k}-\vec{q}}$ irrespective of the value of $\vec{k}$.

### B. Weak-scattering approximation

Using KL as a guide we simultaneously solve Eqs. (14), (16), and (18) in the weak-scattering limit. We consider $H'$ to be weak, with the strength of $H'$ designated by the small parameter $\lambda$. Equation (14) can now be used to show that the diagonal element $f_{\vec{k}\vec{k}}$ is of order $\lambda^0$ and the off-diagonal element $f_{\vec{k}\vec{k}'}$ is of order $\lambda$. To establish this we need to consider the commutator $[\rho, e\vec{x}\cdot\vec{E}]$. KL show that the commutator may be evaluated by introducing the commutation rule $\vec{x}=i\partial/\partial\vec{p}$, where $\vec{p}$ is the electron momentum. This leads immediately to the following expression for the diagonal element to lowest order in $\lambda$. (Refs. 17 and 35):

$$[\rho, e\vec{x}\cdot\vec{E}]_{\vec{k}\vec{k}}=-ie\vec{E}\cdot\left(\frac{\partial\rho_{\vec{k}}}{\partial\vec{k}}\right), \tag{19}$$

where $\rho_{\vec{k}}=\{\exp[(\epsilon_{\vec{k}}-\epsilon_F)/k_BT]+1\}^{-1}$ denotes the Fermi-Dirac distribution.

The off-diagonal ($\vec{k}\neq\vec{k}'$) element of the commutator, again to lowest order, is given by[17,35]

$$[\rho, e\vec{x}\cdot\vec{E}]_{\vec{k}\vec{k}'}=ieEH'_{\vec{k}\vec{k}'}\left(\frac{\partial}{\partial\vec{k}}+\frac{\partial}{\partial\vec{k}'}\right)\left(\frac{\rho_{\vec{k}}-\rho_{\vec{k}'}}{\epsilon_{\vec{k}}-\epsilon_{\vec{k}'}}\right). \tag{20}$$

Now it is apparent that expression (19) is $O(\lambda^0)$ and expression (20) is $O(\lambda)$. Therefore, by Eq. (14), the diagonal element $f_{\vec{k}\vec{k}}$ is $O(\lambda^0)$. Using the KL notation we write $f_{\vec{k}\vec{k}}$ as $f_{\vec{k}}$ and use Eqs. (14) and (19) to find that

$$f_{\vec{k}}=e\tau\vec{E}\cdot\left(\frac{\partial\rho_{\vec{k}}}{\partial\vec{k}}\right). \tag{21}$$

It is clear from Eqs. (14) and (20) that the off-diagonal $f_{\vec{k}\vec{k}'}$ begins at $O(\lambda)$. Consequently to obtain $f_{\vec{k}\vec{k}'}$ to $O(\lambda)$, one needs to consider only those terms in the second sum on the right-hand side of Eq. (14) in which the diagonal element $f_{\vec{k}}$ or $f_{\vec{k}'}$ appears. Similarly, since the off-diagonal elements of $\rho$ are $O(\lambda)$ we keep only the diagonal part of $\rho$ in the last term on the right-hand side of Eq. (14). We thus obtain for the off-diagonal elements to $O(\lambda)$, the result

$$f_{\vec{k}\vec{k}'}=f^E_{\vec{k}\vec{k}'}+f^W_{\vec{k}\vec{k}'}+f^S_{\vec{k}\vec{k}'}\,, \tag{22}$$

where

$$f^E_{\vec{k}\vec{k}'}=\frac{[\rho, e\vec{x}\cdot\vec{E}]_{\vec{k}\vec{k}'}}{\epsilon_{\vec{k}}-\epsilon_{\vec{k}'}-i/\tau} \tag{23}$$

is dependent on the electric field explicitly and the commutator is given by expression (20). The second part of $f_{\vec{k}\vec{k}'}$ is given by

$$f^W_{\vec{k}\vec{k}'}=\frac{(f_{\vec{k}}-f_{\vec{k}'})V^Q_{\vec{k}\vec{k}'}}{\epsilon_{\vec{k}}-\epsilon_{\vec{k}'}-i/\tau} \tag{24}$$

and will be shown to be associated with the "electron wind." The third part of $f_{\vec{k}\vec{k}'}$ is given by

$$f^S_{\vec{k}\vec{k}'}=\frac{(\rho_{\vec{k}}-\rho_{\vec{k}'})V^1_{\vec{k}\vec{k}'}}{\epsilon_{\vec{k}}-\epsilon_{\vec{k}}-i/\tau}\,, \tag{25}$$

which explicitly contains that part of the screening potential which is linear in the field. We therefore identify $f^S_{\vec{k}\vec{k}'}$ as the self-consistent screening response to the perturbations $f^E_{\vec{k}\vec{k}'}$ and $f^W_{\vec{k}\vec{k}'}$.

We can now easily determine $n(\vec{q})$ from Eq. (16) and Eqs. (22)–(25). The important step is to replace the matrix element $V^1_{\vec{k},\vec{k}-\vec{q}}$ in $f^S_{\vec{k},\vec{k}-\vec{q}}$ by the right-hand side of the Poisson equation (18).

In analogy with expression (22), we express the result of the calculation as

$$n(\vec{q})=n^E(\vec{q})+n^W(\vec{q})+n^S(\vec{q})\,, \tag{26}$$

where $n^E(\vec{q})=\sum_{\vec{k}} f^E_{\vec{k},\vec{k}-\vec{q}}$ and similarly for $n^W(\vec{q})$ and $n^S(\vec{q})$. It is particularly useful to introduce the explicit form of $n^S(\vec{q})$. From Eq. (25), we have

$$n^S(\vec{q})=q^2[1-\epsilon(q)]V^1(\vec{q})/4\pi e^2\,, \tag{27}$$

where

$$\epsilon(q)=1-\frac{4\pi e^2}{q^2}\sum_{\vec{k}}\frac{\rho_{\vec{k}}-\rho_{\vec{k}-\vec{q}}}{\epsilon_{\vec{k}}-\epsilon_{\vec{k}-\vec{q}}-i/\tau} \tag{28}$$

is the Lindhard dielectric function.[36] When $n^S(\vec{q})$ is eliminated from Eq. (26) by means of Eqs. (27) and (18), we find

$$n(\vec{q}) = [n^E(\vec{q}) + n^W(\vec{q})]/\epsilon(q) . \tag{29}$$

We can numerically determine $n(\vec{q})$ by performing the sums $n^{E,W}(\vec{q}) = \sum_{\vec{k}} f^{E,W}_{\vec{k},\vec{k}-\vec{q}}$. Transforming the sums to integrals and evaluating them, we obtain

$$n(\vec{q}) = -[ieE\tau/2\pi\epsilon(q)]V^0(q)\alpha(q)\cos\phi , \tag{30}$$

where $\alpha(q)$ is a function we have evaluated and $\phi$ is the angle between $\vec{E}$ and $\vec{q}$. We have taken $V^0(\vec{x})$ to be spherically symmetric.

The function $\alpha(q)$ can be separated into an electric-field part $\alpha^E(q)$ and an electron-wind part $\alpha^W(q)$ by writing

$$\alpha(q) = \alpha^E(q) + \alpha^W(q) , \tag{31}$$

where $\alpha^E(q)$ and $n^E(\vec{q})$ satisfy Eq. (30) when they replace $\alpha(q)$ and $n(\vec{q})$, respectively, in that equation. $\alpha^W(q)$ and $n^W(\vec{q})$ are related by Eq. (30) in the same way.

Both $\alpha^E(q)$ and $\alpha^W(q)$ depend on $q$, $\tau$, and the Fermi wave vector $k_F$, but only in combinations of the dimensionless variables $\eta$ and $\xi$, where $\eta = q/k_F$ and $\xi = k_F l$, with $l = k_F\tau/m$ being the mean-free-path. The explicit expressions are

$$\alpha^E(q) = \frac{\xi}{\pi}\left(1 - \frac{\eta^2}{4}\right)\ln\left|\frac{\eta+2}{\eta-2}\right| + \frac{\xi}{2\pi}\left(1 - \frac{\eta^2}{4} + \frac{1}{\eta^2\xi^2}\right) \times \ln\left(\frac{(1-\frac{1}{2}\eta)^2 + 1/\eta^2\xi^2}{(1+\frac{1}{2}\eta)^2 + 1/\eta^2\xi^2}\right) \tag{32}$$

and

$$\alpha^W(q) = \theta(2-\eta) + \frac{1}{\pi}\tan^{-1}\left(\frac{1}{\eta\xi(\frac{1}{2}\eta - 1)}\right) - \frac{1}{\pi}\tan^{-1}\left(\frac{1}{\eta\xi(\frac{1}{2}\eta + 1)}\right), \tag{33}$$

where $\Theta(x) = 1$ for $x \geqslant 0$ and zero for $x < 0$. Values for the $\tan^{-1}$ functions are restricted to lie between $\pm\frac{1}{2}\pi$. Results (32) and (33) follow from Eqs. (20)–(31) with no approximation except for invoking the usual condition that $k_B T \ll \epsilon_F$. Both $\alpha^E(q)$ and $\alpha(q)$ are plotted as a function of $\eta$ for $\xi = 3$, 10, and 100 in Fig. 1.

Equations (30)–(33) together with Eq. (17) give the electron density in the weak-scattering approximation. In the $\xi \gg 1$ limit, $\alpha(q) \rightarrow \Theta(2-\eta)$ and $n(\vec{x})$ take the form of the Bosvieux-Friedel dipole[6] associated with the electron-wind force. See Ref. 12 for a picture of $n(\vec{x})$ as calculated from pseudopotential theory in this $\xi \gg 1$ limit.

### C. Local field and force on an impurity ion

Having determined the electron density, we now turn to calculating the local field and the force on an impurity using Eqs. (3) and (2), respectively. For computations, the latter equations are more conveniently expressed in terms of $n(\vec{q})$ rather than $n(\vec{x})$. For example, Eq. (3) becomes

$$\vec{E}_L(\vec{X}) = \vec{E} + \frac{e}{2\pi^2}\int i\vec{q}\,\frac{n(\vec{q})}{q^2}\exp(i\vec{q}\cdot\vec{X})\,d^3q . \tag{34}$$

Assuming that the scattering potential $V^0$ is spherically symmetric and centered at the origin of $\vec{X}$ space, the angular integrations in Eq. (34) can be performed using the $n(\vec{q})$ expression (30). The local field can then be cast into the from given in Eq. (4), where the explicit expression for the local potential $\Phi(\vec{X})$ is

$$\Phi(\vec{X}) = \left(\frac{e^2\tau\vec{E}\cdot\hat{X}}{\pi^2}\right)\int_0^\infty \alpha(q)\,\frac{V^0(q)}{\epsilon(q)}\,j_1(qX)\,dq . \tag{35}$$

Here $\hat{X} = \vec{X}/|\vec{X}|$ and the Bessel function $j_1$ is defined by $j_1(x) = x^{-2}\sin x - x^{-1}\cos x$.

The force on an impurity ion is of special interest. Expressing the integral in Eq. (2) in $\vec{q}$ space, we obtain

$$\vec{F} = Ze\vec{E} - (2\pi)^{-3}\int i\vec{q}\,n(\vec{q})V^0(q)\epsilon(q)\,d^3q , \tag{36}$$

where we have taken the impurity to be at the origin and have replaced the bare electron-ion

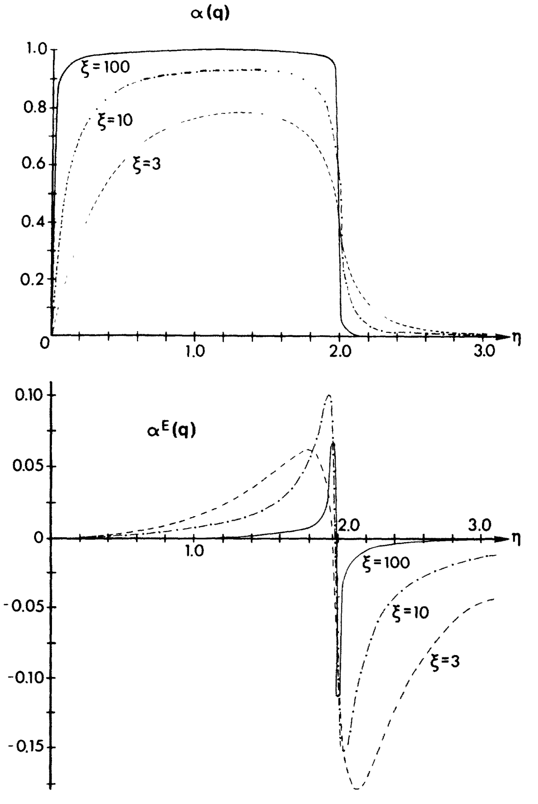

FIG. 1. Functions $\alpha(q)$ and $\alpha^E(q)$ for different values of the parameter $\xi = k_F l$. Variable $\eta$ is $q/k_F$.

interaction $V_0$ by the screened interaction $V^0$ using the linear-screening relation $V_0(q)/\epsilon(q)$.

Taking the expression (30) for $n(\vec{q})$ and performing the angular integration in Eq. (36), we find

$$\vec{F} = Ze\vec{E} - \frac{e\tau\vec{E}}{12\pi^3}\int_0^\infty \alpha(q)\,|V^0(q)|^2 q^3\,dq\,. \tag{37}$$

We have computed the local potential $\Phi(\vec{X})$ and the force $\vec{F}$ using Eqs. (35) and (37), respectively. In our calculations we used the Ashcroft empty-core pseudopotential[37] for $V^0(q)$.[38] Explicitly, we took

$$V^0(q) = -[4\pi e^2 Z/q^2\epsilon(q)]\cos qR_c\,, \tag{38}$$

where $R_c$ is the core radius.

A plot of $\Phi(\vec{X})$ is given in Fig. 2 for $\vec{X}$ along the direction of the electron drift velocity $\vec{v}_D$, where $\vec{v}_D = -e\vec{E}\tau/m$. In this calculation we used the values $k_F = 0.9273$ a.u., $R_c = 1.12$ a.u., and $Z = 3$. These values are appropriate for an aluminum impurity (interstitial) in aluminum metal. The same general features are observed for other choices of these parameters. In the $\xi \gg 1$ regime and at large distances from the impurity ($k_F X \gg 1$), $\Phi(\vec{X})$ varies like $(\hat{E}\cdot\hat{X}/X^2)\sin 2k_F X$. A map of $\Phi(\vec{X})$ in the near-field region is shown in Fig. 3.

The force on an impurity has been evaluated for $k_F$ values appropriate to aluminum ($k_F = 0.9273$ a.u.) and potassium ($k_F = 0.3878$ a.u.) for various values of $R_c$. For convenience, we have taken $Z = 1$ in the impurity pseudopotential expressions (38). The results are shown in Table I for $\xi$-values of 3, 10, and 100. The table gives the electric-field contribution $F^E$ and the electron-wind contribution $F^W$. Here $F^E$ is the contribution from the second term in Eq. (37) when $\alpha^E(q)$ is used in the integrand, and similarly $F^W$ arises from using $\alpha^W(q)$ in the integrand. Note that the wind force $F^W$ dominates, although at smaller $\xi$, the electric-field contribution $F^E$ begins to become appreciable.

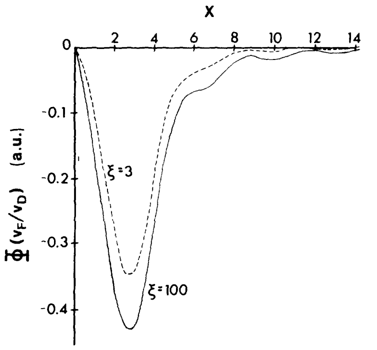

FIG. 2. Local potential near an interstitial aluminum ion during dc transport. The potential is measured at a distance $X$ from the ion and along a vector in the direction of the electron drift velocity $\vec{v}_D$. The distance $X$ is measured in units of $1/k_F$. The quantity plotted is the local potential $\Phi$ multiplied by $(v_F/v_D)$, where $v_F$ is the Fermi velocity. Values are in atomic units. The dashed and full curves correspond to $\xi$ values of 3 and 100, respectively.

## IV. DISCUSSION

### A. Sources of the local field

The contributions to the local field arising from $f^E_{\vec{k}\vec{k}'}$ and $f^W_{\vec{k}\vec{k}'}$ have been associated with the static screening in the external field and with the dynamic screening in the "electron wind," respectively. We investigate this further.

The association of $f^E_{\vec{k}\vec{k}'}$ with the static screening in the electric field was suggested by the presence of $\vec{E}$ in the defining Eq. (23). It turns out that the expression (23) is precisely what one would obtain if one were to compute in $O(\lambda E)$ the change in electron wave functions due to an $e\vec{x}\cdot\vec{E}$ perturbation on the unperturbed plane-wave states in the absence of current flow. Thus $n^E(\vec{x})$ is the $O(\lambda E)$ contribution to static screening, by which we mean screening in the absence of current flow. Note that there is no static screening in $O(\lambda^0 E)$ in our transport problem. Terms of $O(\lambda^0 E)$ appear only in the diagonal element $f_{\vec{k}}$ and not in $f_{\vec{k}\vec{k}'}$ for $\vec{k} \neq \vec{k}'$. The claim made by Sorbello is thus correct[12]: The primary role of the electric field is in setting up the current, or $f_{\vec{k}}$. To allow the electrons locally to screen $\vec{E}$ directly in $O(\lambda^0 E)$ is to double count the response of the electrons to the electric field.

The contribution to the local field arising from $f^W_{\vec{k}\vec{k}'}$ was associated with the electron current or "wind" because of the presence of the current-carrying distribution $f_{\vec{k}}$ in the defining Eq. (24).

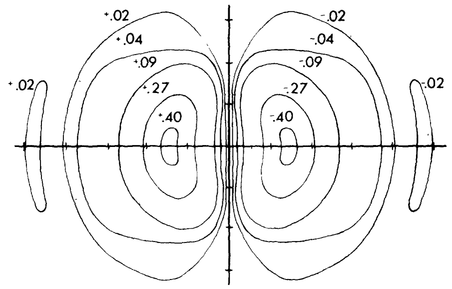

FIG. 3. Equipotential lines for the local potential near an aluminum ion during dc transport. The plane for which the lines are shown is parallel to the electric field and contains the ion at the origin. The electron transport is from left to right. The distance between scale markings on the axes is $2/k_F$. Numerical values are in atomic units and represent the quantity $\Phi(\vec{X}) \times (v_F/v_D)$ for the case of long mean free path ($\xi = 100$).

TABLE I. Forces on an interstitial impurity in aluminum and potassium metal. The force due to the static screening in the electric field is denoted by $F^E$; the force due to the "electron wind" is denoted by $F^W$. Forces are shown for different values of the parameters $\xi$ and $R_c$, where $\xi = k_F l$ and $R_c$ is the pseudopotential core radius. $R_c$ is given in units of $1/k_F$ for aluminum metal and $1/2k_F$ for potassium metal. Positive values for the forces indicate forces in the direction of the electron drift velocity, negative values indicate forces in the direction of the external field. The force units are such that when the values shown are multiplied by the ratio of drift to Fermi velocity $(v_D/v_F)$ one obtains the force in atomic units (double rydberg per Bohr radius). The valence of the impurity ion has been taken to be unity.

| | Aluminum | | | | | | Potassium | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | $\xi=3$ | | $\xi=10$ | | $\xi=100$ | | $\xi=3$ | | $\xi=10$ | | $\xi=100$ | |
| $R_c$ | $F^E$ | $F^W$ | $F^E$ | $F^W$ | $F^E$ | $F^W$ | $F^E$ | $F^W$ | $F^E$ | $F^W$ | $F^E$ | $F^W$ |
| 0.2 | −0.0102 | 0.1216 | −0.0032 | 0.1263 | −0.0004 | 0.1311 | −0.0058 | 0.0369 | −0.0018 | 0.0346 | −0.0003 | 0.0344 |
| 0.4 | −0.0028 | 0.0862 | −0.0004 | 0.0944 | −0.0001 | 0.1003 | −0.0043 | 0.0329 | −0.0013 | 0.0318 | −0.0002 | 0.0319 |
| 0.6 | −0.0008 | 0.0527 | −0.0001 | 0.0590 | −0.0001 | 0.0638 | −0.0026 | 0.0277 | −0.0008 | 0.0277 | −0.0000 | 0.0281 |
| 0.8 | −0.0049 | 0.0338 | −0.0029 | 0.0336 | −0.0002 | 0.0347 | −0.0013 | 0.0219 | −0.0003 | 0.0227 | −0.0000 | 0.0237 |
| 1.0 | −0.0104 | 0.0325 | −0.0039 | 0.0260 | −0.0004 | 0.0231 | −0.0007 | 0.0168 | −0.0002 | 0.0178 | −0.0000 | 0.0188 |
| 1.2 | −0.0128 | 0.0423 | −0.0093 | 0.0389 | −0.0006 | 0.0305 | −0.0007 | 0.0124 | −0.0001 | 0.0132 | −0.0000 | 0.0140 |
| 1.4 | −0.0130 | 0.0586 | −0.0047 | 0.0527 | −0.0008 | 0.0504 | −0.0011 | 0.0095 | −0.0003 | 0.0095 | −0.0000 | 0.0099 |
| 1.6 | −0.0087 | 0.0704 | −0.0028 | 0.0704 | −0.0004 | 0.0720 | −0.0021 | 0.0081 | −0.0006 | 0.0070 | −0.0001 | 0.0068 |
| 1.8 | −0.0043 | 0.0756 | −0.0008 | 0.0811 | −0.0001 | 0.0862 | −0.0032 | 0.0082 | −0.0010 | 0.0059 | −0.0001 | 0.0050 |
| 2.0 | −0.0024 | 0.0744 | +0.0005 | 0.0819 | +0.0004 | 0.0881 | −0.0042 | 0.0093 | −0.0015 | 0.0061 | −0.0002 | 0.0046 |

Moreover, the electron density $n^W(\vec{q})$ is precisely what one would obtain by performing a calculation of the electron density on a coordinate system moving with the electron drift velocity $\vec{v}_D = -e\tau\vec{E}/m$ but with no electric field explicitly present.

To see how $n^W(\vec{q})$ is associated with a calculation in the moving coordinate system, we use Eq. (24) with $f_{\vec{k}}$ and $f_{\vec{k}'}$ described as shifted Fermi-Dirac distributions. That is, we write $f_{\vec{k}} = \rho_{\vec{K}} - \rho_{\vec{k}}$, where $\vec{K} = \vec{k} - m\vec{v}_D$, and similarly for $f_{\vec{k}'}$. [This form is equivalent to Eq. (21) for $\epsilon_F \gg k_B T$.] The charge density $n^W(\vec{q})$ according to rule (16) becomes

$$n^W(\vec{q}) = V^0(q) \sum_{\vec{k}} \frac{\rho_{\vec{K}} - \rho_{\vec{K}-\vec{q}}}{\epsilon_{\vec{K}+m\vec{v}_D} - \epsilon_{\vec{K}-\vec{q}+m\vec{v}_D} - i/\tau} - V^0(q) \sum_{\vec{k}} \frac{\rho_{\vec{k}} - \rho_{\vec{k}-\vec{q}}}{\epsilon_{\vec{k}} - \epsilon_{\vec{k}-\vec{q}} - i/\tau}, \tag{39}$$

where we have changed to a summation over $\vec{K}$ in place of $\vec{k}$ in the first sum. To terms linear in $\vec{v}_D$, the denominator in the first sum is easily expanded to give $\epsilon_{\vec{k}} - \epsilon_{\vec{k}-\vec{q}} - \omega - i/\tau$, where we define $\omega = -\vec{q}\cdot\vec{v}_D$. The first sum is then precisely $q^2[1 - \epsilon(q,\omega)]/4\pi e^2$, where $\epsilon(q,\omega)$ is the frequency-dependent Lindhard function and is given by the $\epsilon(q)$ formula (28) except that $i/\tau$ is replaced by $\omega + i/\tau$ in that formula. Expression (39) is now reduced to

$$n^W(\vec{q}) = V^0(q) q^2[\epsilon(q,0) - \epsilon(q,\omega)]/4\pi e^2 . \tag{40}$$

Since we are keeping only terms linear in $\vec{E}$ or $\vec{v}_D$ throughout our calculation, we can in Eq. (40) make the replacement $\epsilon(q,0) - \epsilon(q,\omega) \to -\omega\partial\epsilon(q,\omega)/\partial\omega$, where the derivative is evaluated at $\omega = 0$. When the resulting $n^W(\vec{q})$ is used in the integral in Eq. (36) for the force, it yields precisely the "drag" or "stopping force" on an impurity moving at velocity $-\vec{v}_D$ in a stationary electron gas.[39] It thus becomes clear that the force arising from $n^W(\vec{q})$ can be thought of as a viscosity or "drag force" which depends on the relative velocity between the electron gas and the impurity. The presence of $\epsilon(q,\omega)$ in Eq. (40) is typical of dynamic screening response.[30]

We can extend our analysis to the more general case of an impurity moving at velocity $\vec{u}$ in an electron gas drifting at velocity $\vec{v}_D$. The potential of the moving impurity is of the form $V^0(\vec{x} - \vec{u}t)$, which introduces an extra time dependence in its Fourier transform, which now becomes $V_0(q)\exp(-i\Omega t)$, where $\Omega = \vec{q}\cdot\vec{u}$. If we now solve the Liouville equation (12) with the ansatz $f \propto e^{-i\Omega t}$, we obtain a consistent solution for $n(q)$ to $O(\lambda u)$ and $O(\lambda v_D)$ provided that we ignore the external-field interaction $e\vec{x}\cdot\vec{E}$. The solution at $t = 0$ can be written $n(\vec{q}) = \tilde{n}^W(\vec{q})/\epsilon(q)$, where

$$\tilde{n}^W(\vec{q}) = V^0(q) q^2[\epsilon(q,0) - \epsilon(q,\omega+\Omega)]/4\pi e^2 \tag{41}$$

plays the role of a new "electron wind" or dynamic screening density. Since $\omega + \Omega = -\vec{q}\cdot(\vec{v}_D - \vec{u})$, Eq. (41) shows that $\vec{v}_D$ and $-\vec{u}$ cause equivalent effects. This equivalence is at the basis of the Das-Peierls[16] "equivalence theorem."

We emphasize, however, that the equivalence between the effects of $\vec{v}_D$ and $-\vec{u}$ is only valid for the $n^W(\vec{q})$ contribution to the local field or force on an impurity. The additional contribution $n^E(\vec{q})$ arising from the commutator $[e\vec{x}\cdot\vec{E}, \rho]$ in the Liouville equation vitiates the "equivalence theorem." However, since the $n^E(\vec{q})$ contribution turns out to be generally small, the "equivalence theorem" holds to a very good approximation in our model. In a more realistic model in which $\tau$ depends on the state $\vec{k}$, the "equivalence theorem" fails due to an additional contribution arising from $\tau_{\vec{K}+m\vec{v}_D}$ in place of $\tau$ in the denominator of the $\vec{K}$ sum in Eq. (39). We are thus in agreement with discussions[16,40] pointing out the importance of a constant relaxation time for the validity of the "equivalence theorem."

### B. Numerical results

Our numerical calculations displayed in Table I show that for $k_F l \gg 1$ the "electron-wind" force dominates the force arising from any static screening in the external field. The origin of this effect can be seen in Fig. 1, where we have plotted $\alpha(q)$ and $\alpha^E(q)$. These quantities when used in Eqs. (35) or (37) give the total screening and static-screening contributions, respectively. Figure 1 implies that $\alpha^E(q)$ is much smaller than $\alpha^W(q)$, except for $q \gtrsim 2k_F$ in the small-$k_F l$ regime. This regime where $k_F l$ is or order unity is not normally achievable for pure metals. Even at the highest temperatures where the ideal resistivity dominates, $k_F l$ is typically around 50. It appears, therefore, that the static-screening contribution will not become comparable to the wind force except for very impure metals.

Note that the force arising from $\alpha^E(q)$ may turn out to be along $\vec{E}$ or opposite to $\vec{E}$, depending on whether the $q > 2k_F$ contribution is larger than the $q < 2k_F$ contribution. The numerical results in Table I show that the $q > 2k_F$ contribution dominates except at higher $R_c$ values. The force due to static screening in the external field, therefore, actually intensifies the field slightly if $R_c$ is not too large. This behavior is contrary to what one would expect for static screening of an external field in thermodynamic equilibrium. The latter behavior does not occur here because the contribution to $n^E$ of $O(\lambda^0 E)$ is missing.

It is also seen from Fig. 1 or from Eqs. (32) and (33) that in the $k_F l \to \infty$ limit, $\alpha^E(q) \to 0$, and $\alpha^W(q) \to \theta(2k_F - q)$. The force obtained in this limit from Eq. (37) is identical to the results obtained previosuly from the ballistic[9,10] and charge-polarization models[6,12] (without static screening of the external field). We note that the $k_F l \to \infty$ limit for $\alpha(q)$ is reached for virtually all $q$ when $k_F l = 100$. However, there are always some significant departures from the $k_F l \to \infty$ limit of $\alpha(q)$ in the neighborhood of $q = 0$ and $2k_F$. The departures around $q = 0$ are not effective in contributing to the integrals of Eqs. (35) or (37), however, because of the phase-space factors $q^3 dq$ at small $q$. The departures around $q = 2k_F$ are also washed away by the integrations. These departures would show up more strongly if the pseudopotential $V^0(q)$ were very sharply peaked (within a $q$ range equal to $l^{-1}$) around $q = 0$ or $2k_F$. This behavior does not occur for pseudopotentials of atomic impurities.

### C. Higher-order contributions: Residual-resistivity dipoles

Within a semiclassical analysis Landauer originally showed that there is a significant contribution to the local field arising from his so-called residual-resistivity dipoles (RRDs).[25] According to later discussions by Landauer[41] and Schaich,[42] the RRD is the electron density arising from the amplitude of the scattered wave functions near the impurity. That is, if we write the total wave function as $\psi(\vec{x}) = \psi_i(\vec{x}) + \psi_s(\vec{x})$, where $\psi_i$ is the incident plane wave and $\psi_s$ is the scattered wave, then the RRD is the dipolarlike charge distribution $-e|\psi_s(\vec{x})|^2$. The RRD is thus $O(\lambda^2)$, or one order higher than we have gone in Sec. III B.

It is straightforward to write the form of the electron density in $O(\lambda^2)$. Denoting this quantity $\delta n(\vec{q})$, we can use Eq. (14) and the rule (16) to deduce that

$$\delta n(\vec{q}) = \delta n^E(\vec{q}) + \delta n^{\mathrm{RRD}}(\vec{q}) + \delta n^O(\vec{q}) + \delta n^S(\vec{q}) , \quad (42)$$

where all terms are electron densities of $O(\lambda^2)$ and linear in $E$. $\delta n^E(\vec{q})$ and $\delta n^{\mathrm{RRD}}(\vec{q})$ arise from the first and second terms, respectively, on the right-hand side of Eq. (14). Both of these terms represent densities which would be set up in an independent-particle picture (no self-consistent screening potential). $\delta n^E(\vec{q})$ is easily found from the expression given by KL[17] for $[\rho, e\vec{x}\cdot\vec{E}]$ to $O(\lambda^2)$. $\delta n^{\mathrm{RRD}}(\vec{q})$ is the RRD electron distribution. It is obtained by using $f^W$ from Eq. (24) in place of the off-diagonal elements of $f$ in the second term on the right-hand side of Eq. (14) and by using the $O(\lambda)$ correction to the diagonal elements of $f$ when they appear in the second term. [There are no such $O(\lambda)$ corrections to $f_{\vec{k}}$ if we choose $V^0_{\vec{k}\vec{k}} = 0$.] $\delta n^O(\vec{q})$ arises from using $f^E$ and $f^S$ from Eqs. (23) and (25) in place of $f$ in this second term of Eq. (14). We also include in $\delta n^O(\vec{q})$ the contribution from the last term of Eq. (14) when the off-diagonal matrix elements of $\rho$ in $O(\lambda)$ are used along with the values of $V^1$ previously calculated in $O(\lambda)$. Finally $\delta n^S(\vec{q})$ arises from using $\rho_{\vec{k}}$ and $\rho_{\vec{k}'}$ for the diagonal elements $\rho_{\vec{k}\vec{k}}$ and $\rho_{\vec{k}'\vec{k}'}$, respectively, in the last term of Eq. (14).

In Eq. (42), $\delta n^S(\vec{q})$ is the self-consistent screening contribution in $O(\lambda^2)$ since it arises from that part of $V^1(q)$ which is $O(\lambda^2)$ in the last term of Eq. (14). Denoting this $O(\lambda^2)$ potential by $\delta V^1(\vec{q})$, the Poisson equation (18) implies that $\delta V^1(\vec{q}) = 4\pi e^2 \delta n(\vec{q})/q^2$. We can now eliminate $\delta n^S(\vec{q})$ in Eq. (42) by combining the Poisson equation and the relation $\delta n^S(\vec{q})=q^2[1-\epsilon(q)]\delta V^1(\vec{q})/4\pi e^2$. In analogy with Eq. (29), we obtain

$$\delta n(\vec{q})=[\delta n^E(\vec{q})+\delta n^{\rm RRD}(\vec{q})+\delta n^O(\vec{q})]/\epsilon(q)\,. \qquad (43)$$

All the terms on the right-hand side are known in terms of explicit $\vec{k}$-space integrals. Unfortunately, these integrals are too complicated to be evaluated analytically. Here we settle for a discussion of the effect of the screening factor $\epsilon(q)$ in Eq. (43). Note that when $\delta n(\vec{q})$ acts on a bare potential $V_0(q)$, the $\epsilon(q)$ factor in Eq. (44) will screen $V_0(q)$. The net effect will be that $\delta n^E$, $\delta n^{\rm RRD}$, and $\delta n^O$ will act on the screened potential $V^0(q)=V_0(q)/\epsilon(q)$ [this can be seen directly from Eqs. (36) and (43) (Refs. 43 and 44)]. As a result of this screening, the force contributed by the RRD on an impurity can be incorporated as a higher-order correction to the pseudopotential $V^0(q)$ in the lower-order expression (37), just as suggested by Schaich.[42]

Now if $\delta n^{\rm RRD}(\vec{x})$ were localized in a finite region of space around the impurity, the screening implicit in the $\epsilon(q)$ factor in Eq. (43) would prevent the creation of any long-range macroscopic polarization field. Instead, the RRD field would be effectively screened out within a distance of the order of a screening length from the region in which $\delta n^{\rm RRD}(\vec{x})$ were localized.[45] This would seem to contradict Landauer's picture[24-26,34] which has the RRDs centered on each impurity and giving rise to an average polarization field, in analogy with classical dielectric theory. Landauer's picture is valid, however, because $\delta n^{\rm RRD}(\vec{x})$ is *not* localized in a finite volume, but rather has the long-range asymptotic form[42] $\hat{E}\cdot\hat{x}/x^2$. The potential due to this extended electron density is not effectively screened out at large distances by the $\epsilon(q)$ factor in Eq. (43).

Since $\delta n^{\rm RRD}(\vec{x})$ is not a localized distribution close to the impurity, estimates[24] which treat the RRD field at the origin as if it were caused by a localized dipolar distribution may be inaccurate. Within a Fermi-Thomas approximation, where $\delta V^1(\vec{x})\propto\delta n(\vec{x})$, it is legitimate to calculate the average macroscopic field due to $\delta n^{\rm RRD}$ by pretending that $\delta V^1(\vec{x})$ is caused by a very localized dipolar charge distribution. This Fermi-Thomas picture is consistent with Landauer's analysis.[25]

Finally we remark that in the $k_F l\to\infty$ limit of Eq. (43), the "electron-wind" related terms are dominant because they involve $f_{\vec{k}}$, which is proportional to $\tau$. In this limit $\delta n^E(\vec{q})$ can be ignored, and $\delta n^O(\vec{q})$ reduces to the nonlinear corrections for the self-consistent-field response to the "electron-wind" charge. Ignoring these nonlinear screening corrections within $\delta n^O(\vec{q})$, we have $\delta n(\vec{q})=\delta n^{\rm RRD}(\vec{q})/\epsilon(q)$, with the RRD now giving the total contribution in $O(\lambda^2)$.

### D. Carrier-density modulation effect

Landauer has pointed out[24] that the local field is influenced by carrier-density modulation[46] (CDM). The CDM effect arises from local changes in the electron density caused by the introduction of the impurity. The density affects the local field by making it easier or harder to overcome the lattice scattering. According to Landauer,[26] the CDM effect would show up as a deviation from Matthiessen's rule by increasing the number of carriers available for conduction. The increase in conductivity, to lowest order in the impurity scattering strength, would be $(\Delta n/n)\sigma_0$, where $\Delta n$ is the number of valence electrons contributed by the impurities and $n$ is the number of conduction electrons originally present. $\sigma_0$ is the conductivity in the absence of the impurities. This addition to the conductivity seems to have been generally ignored by workers in the field presumably because there is a local pile up of $\Delta n$ electrons around the impurities and this localization would seem to disqualify the added carriers from the conduction process. We have found no quantum-mechanical study of this question in the literature. We undertake such a study here.

We trace the CDM effect on the conductivity to the diagonal elements of $[\rho,e\vec{x}\cdot\vec{E}]$ in Eq. (14). The contribution to $[\rho,e\vec{x}\cdot\vec{E}]_{\vec{k}\vec{k}}$ in $O(\lambda)$ is easily obtained from the $\vec{k}\to\vec{k}'$ limit of expression (20).[47] This term plus the $O(\lambda^0)$ contribution from Eq. (19) can be combined and expressed to $O(\lambda)$ as

$$[\rho,e\vec{x}\cdot\vec{E}]_{\vec{k}\vec{k}}=-ie\vec{E}\cdot\left(\frac{\partial\rho'_{\vec{k}}}{\partial\vec{k}}\Big|\right), \qquad (44)$$

where $\rho'_{\vec{k}}=\{\exp[(\epsilon_{\vec{k}}-\epsilon'_F)/k_BT]+1\}^{-1}$ is the Fermi-Dirac distribution appropriate to a new Fermi energy $\epsilon'_F=\epsilon_F-V^0{}_{\vec{k}\vec{k}}$ measured from the band bottom. This shift of the Fermi surface is precisely what one would expect if the extra carriers introduced by the impurities were directly put into the conduction band. It follows that to $O(\lambda)$ the diagonal element $f_{\vec{k}}$ is given by Eq. (21) with $\rho_{\vec{k}}$ replaced by $\rho'_{\vec{k}}$ in that equation. This change in $f_{\vec{k}}$ represents an added current which leads to a conductivity increase $(\Delta n/n)\sigma_0$ exactly as predicted from the CDM effect by Landauer[26] to lowest order in $Z$.

The CDM contribution to the local field $\vec{E}_L$ is difficult to isolate. We have just seen that CDM effects on the conductivity are built into our equations, through an effective shift of $\epsilon_F$. In higher orders of $\lambda$, further corrections to $\epsilon_F$ will occur. These $\epsilon_F$ corrections affect $f_{\vec{k}}$, and will begin to affect $f_{\vec{k}\vec{k}}$, in $O(\lambda^2)$ within the RRD contribution.

We also suggest that some CDM-like contribution may be contained within the term $f^E_{\vec{k}\vec{k}'}$, of Eq. (23). This suggestion is based on the fact that the CDM correction to $f_{\vec{k}}$ is precisely the diagonal element $f^E_{\vec{k}\vec{k}}$. It is natural to expect some vestige of the CDM effect in the off-diagonal elements $f^E_{\vec{k}\vec{k}'}$, and hence in $n^E(\vec{q})$. Note also that $n^E(\vec{q})$, like a CDM contribution, depends explicitly upon the scattering time $\tau$, the screening associated with the potential $V^0$, and the external field $\vec{E}$. However, as we have pointed out, $n^E(\vec{q})$ is more properly interpreted as the static screening response to the external field. Strictly speaking, in the latter interpretation $\tau$ represents the lifetime of the electron states and not a transport scattering time. However, in our model there is no distinction between these two quantities since $\tau$ enters the Liouville equation (12) as a universal relaxation time valid for all perturbations.

Higher-order CDM contributions are still more difficult to isolate. Furthermore, any rigorous calculation of the CDM effect should be done outside the relaxation-time approximation so as to allow for all interference effects between electron-phonon and electron-impurity scattering.[14] We conclude that while certain CDM-like effects are identifiable, it is generally difficult, if not impossible, to separate out from a quantum-mechanical calculation those terms associated with the semiclassical CDM effect. Fortunately, it is not necessary to do this.

## V. CONCLUSION

We have seen that the local electric field can be expressed exactly in terms of the electron density according to Eq. (3). We have evaluated the charge density by solving the Liouville equation in the weak-scattering limit. Our calculation represents the quantum-mechanical generalization of the semiclassical Das-Peierls analysis,[16] and is the first correct Bosvieux-Friedel-type calculation[6,7,12] insofar as no *ad hoc* assumptions are made concerning the static screening of the external field.

The local field, as well as the force on an impurity, contains contributions from the external field, from the static screening in the presence of the external field, and from the dynamic screening in the presence of the electron current or "electron wind." In the $k_F l \gg 1$ regime the "electron-wind" term dominates the static-screening response. There is no screening $O(Z)$. This is in disagreement with the Bosvieux-Friedel analysis,[6] but it is in agreement with the semiclassical analyses of Das and Peierls[16] and Rorschach.[48] Our result is also in agreement with the work of Kumar and Sorbello[13] and Sham[14] who used linear-response theory for an interacting electron gas.[13,14] The contribution which we have denoted by the term "static screening" is not present in the final linear-response expressions,[13-15] but this contribution is negligible in the $k_F l \gg 1$ regime. In general, this contribution does not necessarily weaken the electric field at the impurity; in certain situations, it may actually intensify the local field. For this reason, it may be preferable to abandon the term "static-screening" contribution in favor of the somewhat less suggestive term "electrostatic" contribution.

Our calculations have been performed in the weak-scattering limit, i. e., to lowest order in the pseudopotential.[38] This is formally equivalent to performing the calculations to the leading order in $Z$. However, it is argued that the validity of lowest-order pseudopotential theory for impurity scattering is not limited to the $Z \leq 1$ regime.[49,50]

We have considered contributions which are higher order in the electron-impurity interaction. Specifically, we found that Landauer's residual-resistivity dipoles[25] contribute to the local field near an impurity and give rise to long-range macroscopic fields. These fields are not screened out because of the extended nature of the dipolar charge.

Our calculations show that Landauer's carrier-density modulation effect contributes to the local field in higher orders of the impurity-scattering pseudopotential. The CDM effect contributes to the conductivity by shifting the Fermi energy with respect to the band bottom. The number of carriers taking part in the conduction process is effectively augmented by the number of valence electrons brought in by the impurities. The resulting increase in conductivity is in agreement with recent estimates by Landauer.[26]

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*Research sponsored by the Air Force Office of Scientific Research, Air Force Systems Command, USAF, under Grant No. AFOSR-76-3082.

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[29] The net force on the nucleus of an isolated ion in free space is $Ze\vec{E}$. This force is produced by the sum of the core-polarization field and the external field. It follows that the field at the nucleus due to core polarization is $(Z/A-1)\vec{E}$, where $A$ is the atomic number.

[30] D. Pines and P. Nozières, *The Theory of Quantum Liquids* (Benjamin, New York, 1966), Vol. I, Chap. 3.

[31] S. Doniach and E. H. Sondheimer, *Green's Functions for Solid State Physicists* (Benjamin, Reading, Mass., 1974).

[32] The integral in Eq. (3) will generally depend on the geometry even for a very large metal sample since there are geometry-dependent surface charges at the metal-electrode interface at the sample boundary. This means that unless some boundary condition is prescribed, the value of the integral is ill defined in the limit $\Omega\rightarrow\infty$, where $\Omega$ is the sample volume. The boundary condition we are assuming is the no-screening condition discussed earlier, i.e., we are allowing no surface polarization-charge at the sample boundary as $\Omega\rightarrow\infty$. This is consistent with the periodic boundary conditions of Ref. 17 and the transverse field assumed in Ref. 31.

[33] An advantage of visualizing the transport problem in a finite toroidal geometry, is that the hermiticity of operators is preserved. It has been pointed out by Rorschach (private communication) that for the scattering problem in an infinite medium, there are corrections to equations of motion due to the non-Hermiticity of $\mathcal{H}$ with respect to scattering states. (There are contributions from incident and scattered wavefunctions at infinity.) This difficulty does not exist for a finite system such as the toroidal model, or of course, the real physical circuit. For the latter, $\mathcal{H}$ is Hermitian but generally very complicated due to such external details as the battery and connecting wires. One can argue, however, that there is no direct interaction in $\mathcal{H}$ between the test particle at $\vec{X}$ and the external complications. This implies that there are no direct contributions from the latter in the equation of motion from which Eq. (2) is derived. One again arrives at Eq. (2) but now $n(\vec{x})$ is to be computed in the presence of the full Hamiltonian $\mathcal{H}$. One can then argue that the external complications do not affect $n(\vec{x})$ near the impurity and arrive at Eq. (2) without explicitly considering the external complications.

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[44] The effective screening of $\delta n^{\mathrm{RRD}}$ occurs in Sham's work (Ref. 14) when he follows Langer's prescription

(Ref. 20) and dresses all bare interaction lines with the dielectric function.

[45] Any localized-charge distribution $\Delta n(\vec{x})$ will give rise to a potential which is screened out due to the dielectric screening described by $\epsilon(q)$. For example, if $\Delta n(\vec{x})$ is point charge at $\vec{x}=0$, then within a Fermi-Thomas approximation the potential will decay like $x^{-1}\exp(-x/a)$, where $a$ is the screening length. By superposition, similar decaying behavior is obtained outside any region where $\Delta n(\vec{x})$ is localized. [The Lindhard response gives Friedel oscillations rather than exponential decay, of course, but for localized $\Delta n(\vec{x})$, the long-range dipolar fields are effectively screened out.]

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