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Electromigration and the local transport field in mesoscopic systems

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An analysis is presented for the local field and electromigration driving force in mesoscopic systems, i.e., systems in which the dimension along the transport direction is smaller than the electron mean free path due to inelastic scattering. The electromigration driving force is a measure of the microscopic electric field acting on an impurity, and, in general, consists of two contributions, namely, the "electron-wind force" and the "direct force." The local transport field also consists of electron-wind and direct contributions. Detailed analyses are presented for the local fields, forces, and resistivities in the following mesoscopic systems: (i) one-dimensional (1D) disordered conductors; (ii) an impurity-layer or grain boundary sandwiched between reservoirs; and (iii) an impurity in the vicinity of a point contact. For the first two systems, the direct force and the associated direct field vanish, whereas in the point-contact system the wind and direct contributions are comparable. The net electromigration force on a 1D conductor is a measure of the true potential drop across the disordered region, and is proportional to the Landauer resistivity. In the case of an isotropically scattering impurity near a point contact, the wind force is proportional to the impurity-induced change in the contact resistivity. Inconsistencies are pointed out in the use of linear-response formalism based upon the existence of an external field in mesoscopic systems.

I. INTRODUCTION

Electron transport in metals containing defects is characterized by strong inhomogeneities in the microscopic electric field near the defects. The nature of these inhomogeneities in the transport field was first described by Landauer in his classic 1957 paper.[1] Besides their importance in the electronic conduction problem, these field inhomogeneities play a central role in the theory of electromigration,[2,3] which is the phenomenon of atomic migration in the presence of electron transport. It is for this reason that theorists working on electromigration have delved more deeply into the nature of electric field inhomogeneities near defects.[4–17]

Recently, interest in microscopic electric-field inhomogeneities has been reawakened by intense activity in the study of electron transport phenomena in mesoscopic systems.[18–27] In such systems, which occupy the middle ground between the atomic and macroscopic length scales, the microscopic electric field can, in principle, be probed experimentally. However, in typical experimental configurations, it appears that the field measurement is strongly affected by the voltage probes themselves.[19] In this paper we investigate the nature of the local field in mesoscopic systems and explore the possibility of using electromigration as a probe of the local field.

We shall consider the microscopic electric field within the framework of the local-field method discussed by Chu and Sorbello.[17] The method is based on ideas contained in Landauer's 1957 paper, with the addition of further insights obtained from electromigration theory. In particular, we separate the local electric field in the vicinity of an impurity (or a more general defect) into two parts. One part is associated with the electronic distribution $g_{\mathbf{k}}$ incident upon the impurity and the other part is associated with the direct action of the long-range electric field $\mathbf{E}_0$ at the impurity. Using electromigration terminology,[2,3] the part associated with $g_{\mathbf{k}}$ is called an "electron-wind" contribution, and the part associated with $\mathbf{E}_0$ is called a "direct" contribution.

As far as the electromigration force on an impurity is concerned, there is general agreement that the force due to the electron wind equals the rate of momentum transfer to the impurity from the scattered electrons. The direct force, or the force exerted on the impurity by $\mathbf{E}_0$, has always been controversial,[2,3] and the most definitive treatments, whether semiclassical[9] or quantum mechanical,[14] are not easy to follow. In these treatments, one assumes the existence of a uniform $\mathbf{E}_0$, and effectively calculates the resulting dynamical polarization in the vicinity of the impurity. The force can be expressed as $Z_d e \mathbf{E}_0$, where Z_d is an effective valence for the direct force. Thus, there are two aspects of the direct-force problem, namely: finding $\mathbf{E}_0$ and finding Z_d. We shall accept out previous determination of Z_d,[14] and in this paper, we instead focus our attention on $\mathbf{E}_0$. In bulk systems, $\mathbf{E}_0$ can be taken to equal the average or macroscopic field. However, this is not the case in mesoscopic systems, where one must be very careful in identifying the appropriate sources of $\mathbf{E}_0$. For example, in the one-dimensional conductor (treated in Sec. III A), one must take $\mathbf{E}_0=0$ despite the existence of an overall average electric field across the system. The key point is that the average field is set up by the self-consistently screened response to the electron wind. There is no direct field in this case.

In our approach to the conductivity-electromigration problem, we follow Landauer[1] and focus on a small region of radius R containing the impurities, where R is substantially smaller than the background mean free path, l. The various contributions to fields and forces within this near-field region are calculated from the self-consistent electronic response to the external field $\mathbf{E}_0$ and to the incident current. In the case of bulklike systems, one could then describe the conductivity problem from the bottom up, i.e., the fields generated by sources within R would then be added together to yield the correct volume average field, from which the conductivity could be calculated.[1] This is in contrast to the top-down approach within the usual Kubo formalism, where a uniform external field is assumed to be applied across the entire macroscopic system. A Green's function evaluation of Kubo response formulas causes the close-in details (within R) to emerge in various Feynman diagrams.[10,11,13] Yet, for all its elegance, the usual Kubo approach, which assumes a uniform external field, is not quite rigorous. The major problem (in the case of a defect-dominated system) is that there really is no external field. Rather there is a macroscopic average field arising from localized dipolar sources at the defects. This is the central lesson of Landauer's 1957 paper.[1] Assuming a uniform driving field amounts to a kind of mean-field picture, i.e., the microscopic response is calculated by taking the average field as the causal agent. We mention this, not as a criticism of the Kubo approach, but as a caveat that subtle approximations can be implicitly introduced when employing so-called "exact" Kubo formulas. Some of the difficult self-consistency questions with which one is immediately confronted in the bottom-up local-field approach are in fact hidden approximations in the usual Kubo approach. Thus, in principle, the local-field method is not less exact than a Kubo approach.

In the case of mesoscopic systems placed between reservoirs in the Landauer configuration[28,29] (see Sec. III) the local-field method is easier to apply and more soundly based than is the Kubo approach. In retrospect, attempts to rigorously derive the Landauer formula [Eq. (32)] from the Kubo approach[19,26,27] are less a test of the Landauer formula than of the Kubo approach. Of course, one can improve upon the usual Kubo approach and regard the external field to be microscopically inhomogeneous.[19,26,30] But unless the latter is replaced by the true self-consistent field, the approach is again not quite rigorous. Furthermore, if the unknown selfconsistent field is employed as a driving force in the Kubo formalism, we are effectively back to the bottom-up local-field approach.[31] In these remarks, we are in agreement with Landauer's caveat[20,21] on the uncritical application of Kubo formulas.

In the next section we employ the local-field approach and relate the microscopic electric field to the driving force for electromigration. A good deal of this is a summary and critique of the relevant theory for bulk systems. We do, however, introduce some refinements into the theory and discuss the modifications that arise in the study of mesoscopic systems. In Sec. III applications are made to the following specific systems: One-dimensional disordered conductors (Sec. III A); an impurity layer or grain boundary sandwiched between reservoirs (Sec. III B); and an impurity near a point contact (Sec. III C). Further discussion is given in Sec. IV.

II. LOCAL ELECTRIC FIELD AND DRIVING FORCE FOR ELECTROMIGRATION

Previous work exploring the connection between local electric fields and electromigration has focused on bulk-like systems,[8,9,12,16,17] where the length of the system along the transport direction is much larger than the electron mean free path. In that case, a steady-state situation is established in which the electron distribution is governed by background scattering. Within a free-electron-gas model, the background scattering leads to an electronic distribution, $g_{\mathbf{k}}$, of the form

$$(g_{\mathbf{k}})_{\text{bulk}} = -\tau e \mathbf{v}_{\mathbf{k}} \cdot \mathbf{E}_0 \delta(\varepsilon_k - \varepsilon_F) , \tag{1}$$

where τ is the electronic relaxation time associated with background scattering, $\mathbf{v}_{\mathbf{k}} = \hbar \mathbf{k}/m$ is the velocity of an electron in state $\mathbf{k}$, and $\varepsilon_k = \hbar^2 k^2/2m$ is the corresponding energy. m is the electron mass, ε_F is the Fermi energy, and $\mathbf{E}_0$ is the macroscopic electric field. Within this model, the electronic charge current $\mathbf{J}_0$ is given by

$$\mathbf{J}_0 = \mathbf{E}_0/\rho_0 , \tag{2}$$

where $\rho_0 = m/n_0 e^2 \tau$ is the resistivity, with n_0 being the conduction electron density and e the magnitude of the electron charge. We are restricting our attention to temperatures well below the Fermi temperature (ε_F/k_B), which is the appropriate regime for the metallic systems under consideration.

We now consider a single impurity placed in the electron gas. The impurity is exposed to the electron distribution $g_{\mathbf{k}}$ and to the electric field $\mathbf{E}_0$. For the moment we ignore the latter, and consider the effects due to the scattering of electrons in the distribution $g_{\mathbf{k}}$. The electron scattering gives rise to an electron density perturbation, $\delta n_w(\mathbf{r})$, where[11,15,17]

$$\delta n_w(\mathbf{r}) = \sum_{\mathbf{k}} g_{\mathbf{k}} |\psi_{\mathbf{k}}^{(+)}(\mathbf{r})|^2 \tag{3}$$

and $\psi_{\mathbf{k}}^{(+)}(\mathbf{r})$ denotes the scattering state wave function for an electron incident in state $\mathbf{k}$. Note that δn_w is an electron-wind term in that it is set up by the scattering of electrons impinging upon the impurity. (We shall use the subscript w to denote quantities associated with the electron wind.)

The charge pileup described by $\delta n_w(\mathbf{r})$ must be screened self-consistently.[1,15,17] Since $\delta n_w(\mathbf{r})$ effectively acts as a source term in a screening calculation, the final self-consistent potential $\delta\Phi$ can be related to δn_w, via a linear-response screening kernel. In general

$$\delta\Phi(\mathbf{r}) = -e \int K(\mathbf{r},\mathbf{r}') \delta n_w(\mathbf{r}') d^3 r' , \tag{4}$$

where the kernel $K(\mathbf{r},\mathbf{r}')$ gives the self-consistent potential at point $\mathbf{r}$ when a weak point charge is placed at point $\mathbf{r}'$ in an *equilibrium* electron gas. K is obtained from a purely electrostatic quantum-mechanical screening calculation for the system in the absence of transport (but in the presence of the impurity). In writing Eq. (4) we are only assuming linear response in the strength of the macroscopic field. Henceforth, we shall confine our attention to this regime in which local fields and forces are linear in the macroscopic field $\mathbf{E}_0$ or transport current $\mathbf{J}_0$. [More generally, for Eq. (4) to be valid we need only require $\delta\Phi$ to be a linear functional of $g_{\mathbf{k}}$.]

The response kernel K has yet to be calculated for self-consistent screening in the presence of a realistic impurity potential and background scattering. However at distances beyond a few screening lengths from the impurity, we can invoke a Thomas-Fermi approximation, in which case Eq. (4) simplifies to[1,15]

$$\delta\Phi(\mathbf{r}) = -\frac{1}{e}\left[\frac{dn}{dE}\right]^{-1}\delta n_w(\mathbf{r})\ , \tag{5}$$

where dn/dE is the electron density of states at the Fermi level. This is an excellent approximation for the potential averaged over a volume of radius equal to a few screening lengths about point $\mathbf{r}$.[15]

In the asymptotic quantum mechanical region, i.e., for $l \gg r \gg k_F^{-1}$, where k_F is the Fermi wave vector and $l = \hbar k_F \tau/m$ is the mean free path, the potential is readily evaluated from Eqs. (3) and (5). The result is the Landauer residual-resistivity-dipole field, namely[1,15,16]

$$\delta\Phi(\mathbf{r}) \sim -\frac{p\cos\theta}{r^2}\ , \tag{6}$$

where we have chosen the impurity to be at the origin and θ is the angle between $\mathbf{r}$ and $\mathbf{E}_0$. The magnitude of the dipole moment p is given by $3\pi\hbar J_0 S_0/4k_F^2 e^2$, where S_0 is the scattering transport cross section.[1,16] Equation (6) can be obtained from Eqs. (3) and (5) by substituting into Eq. (3) the asymptotic form of $\psi_{\mathbf{k}}^{(+)}(\mathbf{r})$, namely

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{r}) = \Omega^{-1/2}[\exp(i\mathbf{k}\cdot\mathbf{r}) + r^{-1}f(\theta')\exp(ikr)]$$

where Ω is the volume. Subsequent summation over $\mathbf{k}$ and spatially averaging over a window of a few wavelengths in size so as to eliminate Friedel oscillations[15] leads to expression (6).

Further calculation is required to determine $\delta\Phi(\mathbf{r})$ in the extreme far-field region where $r > l$.[1,17] No one has yet succeeded in treating this problem fully, including the combined effects of coherent and incoherent scattering away from the impurity. However, for the case of an impurity in a bulk system, a semiclassical transport equation approach[1,17] for $r > l$ again leads to expression (6). Fortunately, for the mesoscopic systems considered here, solutions in the region $r > l$ are not required. In this respect, a mesoscopic system is simpler than a bulklike system.

Thus far we have considered the contribution to the local field arising from the electron wind, i.e., from the incident $g_{\mathbf{k}}$ distribution. We now turn to the role played by the field $\mathbf{E}_0$ at the impurity. We expect $\mathbf{E}_0$ to cause some local polarization of the electron cloud around the impurity, which will modify the local electric field in the vicinity of the impurity. This represents a direct action by the field $\mathbf{E}_0$, rather than the indirect action of $\mathbf{E}_0$ via the establishment of $g_{\mathbf{k}}$. Adopting terminology from electromigration theory,[2,3] we refer to this as a direct-field effect.

Landauer has described the role of the direct field in terms of a carrier-density modulation effect.[9] In its simplest form, his idea is that the conduction-electron screening cloud which surrounds an attractive impurity in equilibrium (no transport) modulates the net conductivity of the background scattering by increasing the local electron density. This results in a local increase in conductivity, which in turn, results in a local decrease of the E field so that current continuity through the impurity potential be preserved. The net effect is an overall correction to the impurity resistivity, or a deviation from Mathiessen's rule. Note that the local field at the impurity due to the presence of E_0 is on the order of E_0, whereas the local fields associated with electron-wind contributions in bulklike systems are usually much larger than this. This is because wind contributions, being linear in $g_{\mathbf{k}}$ are of order $k_F l E_0$ [see Eq. (1)], and for good bulk conductors, $k_F l \gg 1$. In mesoscopic systems, on the other hand, $g_{\mathbf{k}}$ is in general no longer given by Eq. (1), so that these estimates do not apply.

We now consider aspects of the theory of electromigration which relate to the problem under consideration. To keep the discussion relatively simple, we describe the impurity within the point-core model.[32] That is, the bare potential V_b is taken to be

$$V_b(\mathbf{r}) = -\frac{Ze^2}{|\mathbf{r}-\mathbf{r}_0|}\ , \tag{7}$$

where $\mathbf{r}_0$ is the position of the impurity, and Z is the bare valence. The total self-consistent screened potential in the absence of transport is denoted by $V(\mathbf{r})$, which for later convenience we write in terms of an unknown function $H(\mathbf{r},\mathbf{r}_0)$ as follows:

$$V(\mathbf{r}) = -Ze^2 H(\mathbf{r},\mathbf{r}_0) \tag{8}$$

The point-core model assumes that the core electrons are confined to a region of dimensions much smaller than a Fermi wavelength. In the case of hydrogen in those metals for which no bound states of hydrogen occur, the bare potential (7) with $Z = 1$ is essentially exact.

The force, $\mathbf{F}(\mathbf{r}_0)$, exerted on an impurity ion at position $\mathbf{r}_0$ is given by the local electric field acting on the ion. That is,[12]

$$\mathbf{F}(\mathbf{r}_0) = Ze\mathbf{E}_L(\mathbf{r})|_{\mathbf{r}=\mathbf{r}_0}\ , \tag{9}$$

where $\mathbf{E}_L(\mathbf{r})$ is the true local field at position $\mathbf{r}$ in the presence of the impurity at $\mathbf{r}_0$. Since we are interested only in transport fields and forces, $\mathbf{F}$ and $\mathbf{E}_L$ refer to quantities that are linear in the macroscopic field or current. Note that the impurity is acting as a built-in probe of the local electric field $\mathbf{E}_L(\mathbf{r})$. It must be emphasized however that the field probed by the impurity is the field that exists at the impurity *in the presence of the impurity*. If we imagine that $Z \to 0$, then of course the impurity would measure the field $\mathbf{E}_0$ appropriate to the system in the absence of the impurity. This follows from the fact that $\mathbf{E}_L(\mathbf{r}_0) = \mathbf{E}_0 + O(Z)$. In this limit the impurity is acting like the classical external charge probe

$Q=Ze$, where $Q\rightarrow 0$, as envisioned in the operational definition of the electric field in classical electrostatics.

Explicitly, the local electric field depends upon the net electron density $\delta n(\mathbf{r})$ according to

$$\mathbf{E}_L(\mathbf{r})=\mathbf{E}_0(\mathbf{r})+e\nabla\int\frac{\delta n(\mathbf{r}')d^3r'}{|\mathbf{r}-\mathbf{r}'|}\ , \tag{10}$$

where the density integral follows from the operator definition of the electric field. $\delta n(\mathbf{r})$ is the net perturbed density, including wind, direct, and screening contributions. Combining Eqs. (9) and (10), and the definition (7), we obtain

$$\mathbf{F}(\mathbf{r}_0)=ZeE_0(\mathbf{r}_0)-\int\delta n(\mathbf{r})\frac{\partial V_b}{\partial\mathbf{r}_0}d^3r\ , \tag{11}$$

which is recognized to be the quantum-mechanical expectation value of the force operator in linear response.[7] That is, $\mathbf{F}(\mathbf{r}_0)=\langle\Psi|-\partial\mathcal{H}/\partial\mathbf{r}_0|\Psi\rangle$ evaluated to first order in $\mathbf{E}_0$ where $|\Psi\rangle$ is the exact many-body nonequilibrium state of the system, and $\mathcal{H}$ is the system Hamiltonian including the interaction with the external field $\mathbf{E}_0$.

The net perturbed electron density $\delta n(\mathbf{r})$ can be expressed as

$$\delta n(\mathbf{r})=\delta n_w(\mathbf{r})+\delta n_d(\mathbf{r})+\delta n_s(\mathbf{r})\ , \tag{12}$$

where δn_w and δn_d are the unscreened densities associated with wind and direct effects,[33] and δn_s is the additional electron screening density which is induced in response to $\delta n_w+\delta n_d$. An expression for the self-consistent potential arising from $\delta n_w+\delta n_d$ follows from the extension of Eq. (4) to include the δn_d contribution, viz.,

$$\delta\Phi(\mathbf{r})=-e\int K(\mathbf{r},\mathbf{r}')[\delta n_w(\mathbf{r}')+\delta n_d(\mathbf{r}')]d^3r'\ . \tag{13}$$

The density δn can then be determined from Eq. (13) and the Poisson equation

$$\delta n(\mathbf{r})=\frac{1}{4\pi e}\nabla^2\delta\Phi(\mathbf{r})\ . \tag{14}$$

The use of Eqs. (13) and (14) in Eq. (11) yields the force expression

$$\mathbf{F}(\mathbf{r}_0)=\mathbf{F}_w(\mathbf{r}_0)+\mathbf{F}_d(\mathbf{r}_0)\ , \tag{15}$$

where

$$\mathbf{F}_w(\mathbf{r}_0)=\frac{1}{4\pi}\int\nabla_{\mathbf{r}}^2K(\mathbf{r},\mathbf{r}')\delta n_w(\mathbf{r}')\frac{\partial V_b(\mathbf{r})}{\partial\mathbf{r}_0}d^3r\,d^3r' \tag{16}$$

and

$$F_d(\mathbf{r}_0)=Ze\mathbf{E}_0(\mathbf{r}_0)+\frac{1}{4\pi}\int\nabla_{\mathbf{r}}^2K(\mathbf{r},\mathbf{r}')\delta n_d(\mathbf{r}')\frac{\partial V_b(\mathbf{r})}{\partial\mathbf{r}_0}d^3r\,d^3r'\ . \tag{17}$$

These force expressions can be simplified by making use of the following reasonable scheme for the screening response. Imagine breaking up V_{bare} into small elements ΔV_{bare}, and allow the electron gas to screen each element independently. Thus the Fourier-transformed screened elements are $\Delta V(\mathbf{q})=\Delta V_{\text{bare}}(\mathbf{q})/\varepsilon(\mathbf{q})$, where $\varepsilon(\mathbf{q})$ is the dielectric function. The quantum-mechanical problem is then solved to all orders in the screened elements $\Delta V(\mathbf{q})$, including multiple scattering between screened elements. In this picture, the screening kernel K in Eqs. (16) and (17) reduces to its linear-response form, namely $K_{\mathbf{q}\mathbf{q}'}=[4\pi/q^2\varepsilon(\mathbf{q})]\delta_{\mathbf{q}\mathbf{q}'}$. Using this Fourier-transform expression of the kernel in the evaluation of Eqs. (16) and (17) yields

$$\mathbf{F}_w(\mathbf{r}_0)=-\int\delta n_w(\mathbf{r})\frac{\partial V}{\partial\mathbf{r}_0}d^3r\ , \tag{18}$$

$$\mathbf{F}_d(\mathbf{r}_0)=Ze\mathbf{E}_0-\int\delta n_d(\mathbf{r})\frac{\partial V}{\partial\mathbf{r}_0}d^3r\ , \tag{19}$$

where V is the screened response, and, for the point-core model is given by Eq. (8) with H replaced by K in that equation. Note, however, that expressions (18) and (19) are valid for arbitrary impurity potentials within the screening approximation scheme we have described. Equation (18) has been the starting point for rather sophisticated wind-force calculations.[34–36]

Equations (18) and (19) are very useful in that they allow the force (and the local field) to be calculated from an assumed form for the equilibrium impurity-potential V without the necessity of performing a full self-consistent-screening calculation for $\delta n(\mathbf{r})$. The quantities to be calculated are $\delta n_w(\mathbf{r})$ and $\delta n_d(\mathbf{r})$, which are set up by exposing the screened potential V to an incident electron current $g_{\mathbf{k}}$ and a field $\mathbf{E}_0$, respectively. Stated another way, we can calculate the force by treating the electrons as noninteracting among themselves but interacting with the external field $\mathbf{E}_0$, the screened potential V, and the background scatterers. The problem has thus been reduced to independent-particle response. Of course, one could have invoked an independent particle picture at the outset, and, from it, attempt to deduce Eqs. (18) and (19). In such a picture V is a prescribed potential seen by noninteracting electrons, and the force on the impurity due to the electron response is calculated by assuming that the impurity is a rigid, neutral entity comprised of the sources of V (core plus screening charges). In this picture, δn and V_b in Eq. (11) would be replaced by $(\delta n_w+\delta n_d)$ and V, respectively, leading at once to Eqs. (18) and (19). Note, however, that the external force contribution $Ze\mathbf{E}_0(\mathbf{r}_0)$ must remain as is in Eq. (11). The impurity must not be regarded as a rigid, neutral entity as far as the external field $\mathbf{E}_0$ is concerned. Our detailed self-consistent screening derivation of Eqs. (18) and (19) shows that this is the case. Furthermore, by employing a self-consistent screening approach, we have transcended the independent-particle picture in that we are able to obtain the true local electric field, $\mathbf{E}_L$. The latter is obtained by dividing the force by Ze, according to Eq. (9). Also, as we shall see, our approach leads to a clearer picture of the external field $\mathbf{E}_0$. This will turn out to be a crucial point in our treatment of mesoscopic systems.

The force due to the electron wind can also be evaluated directly from the rate of momentum transfer by the electrons to the impurity,[37,38] viz.,

$$\mathbf{F}_w(\mathbf{r}_0)=\sum_{\mathbf{k}\mathbf{k}'}\hbar(\mathbf{k}-\mathbf{k}')P_{\mathbf{k}\mathbf{k}'}g_{\mathbf{k}}\ , \tag{20}$$

where $P_{\mathbf{k}\mathbf{k}'}$ is the transitional probability (probability per unit time) for an electron being scattered (elastically) from state $\mathbf{k}$ to state $\mathbf{k}'$ by the impurity. The equivalence of expressions (18) and (20) within an independent particle picture is obvious; these expressions are simply alternate ways of calculating the expectation value of the force operator $(i/\hbar)[\mathbf{p},H]$, where $H=p^2/2m+V$ and $\mathbf{p}$ is the electron momentum operator. We remark that expressions (18) and (20) are equivalent for an isolated impurity in a free electron gas. In more general cases, it may not be possible to express the momentum transfer to the impurity as in expression (20). This is the situation when the electrons are not free or when more than one impurity is involved in the scattering process. In such cases, however, Eq. (18) remains valid.

The direct force on the impurity ion due to the external field is denoted by $\mathbf{F}_d(\mathbf{r}_0)$ and can be written as

$$\mathbf{F}_d(\mathbf{r}_0)=Z_d e\mathbf{E}_0(\mathbf{r}_0)\ , \tag{21}$$

where Z_d is the effective valence for the direct force,[2,3,9,14] and $\mathbf{E}_0(\mathbf{r}_0)$ is the "external field" at the position of the impurity ion. Here "external" means that the field $\mathbf{E}_0(\mathbf{r}_0)$ arises from sources external to the impurity in question, i.e., it is set up by processes that occur in the absence of the impurity at $\mathbf{r}_0$. Further care is required in defining $\mathbf{E}_0(\mathbf{r}_0)$ when there is more than one impurity present in the system. Consider a cluster of impurities, and let the quantum-mechanical scattering states $\psi_{\mathbf{k}}^{(+)}(\mathbf{r})$ pertain to scattering by the entire cluster. Now $\delta n_w(\mathbf{r})$ calculated from Eq. (3), and screened via Eq. (4), contains the sum of residual-resistivity-dipole fields [see expression (6)] centered at each of the other impurities and acting on the impurity in question at $\mathbf{r}_0$. Since this total field represents a properly screened quantum-mechanical response, it should not be included an additional time as an external field. We conclude that, in the general case, $\mathbf{E}_0(\mathbf{r}_0)$ is the electric field at $\mathbf{r}_0$ due to all agents external to the quantum-mechanical scattering problem which is being considered for $\psi_{\mathbf{k}}^{(+)}(\mathbf{r})$. Thus $\mathbf{E}_0(\mathbf{r}_0)$ is the field that exists when the potential of the impurity cluster is set to zero. For impurities in a bulk system, $\mathbf{E}_0$ can be taken to be the average or macroscopic field; but, for mesoscopic systems this is not correct.

The existence of Z_d has been a controversial issue in electromigration theory.[2,3] Bosvieux and Friedel[4(a)] (and their followers[4(b)]) argued that $Z_d=0$, while others[2,5,10] have argued that $Z_d=Z$. However, as shown by Landauer[9] in a semiclassical analysis and by Rimbey and Sorbello[13,14] in a quantum-mechanical analysis, the value of Z_d depends on the details of the impurity potential V. In the weak-scattering limit, it is found that $Z_d\approx Z$, or more formally, $Z_d=Z+O(Z^2)$. For a pseudopotential model of a scatterer, it is presumably a good approximation to invoke the weak-scattering limit and take $Z_d\approx Z$. A general quantum-mechanical expression for Z_d in terms of the one-electron Green function for a single impurity is given in Ref. 14, along with a model calculation for hydrogen in metals. Values of Z_d on the order of unity were found.[14]

The additional resistivity $\delta\rho$ due to an impurity is expected to be related to the wind force since both quantities are a measure of the scattering cross section. To explore this relationship, we cast expression (20) in the form

$$\mathbf{F}_w(\mathbf{r}_0)=\sum_{\mathbf{k}}\frac{\hbar\mathbf{k}}{\tau_{\text{imp}}}g_{\mathbf{k}}\ , \tag{22}$$

where

$$\frac{1}{\tau_{\text{imp}}}=\sum_{\mathbf{k}'}[1-\cos(\mathbf{k},\mathbf{k}')]P_{\mathbf{k}\mathbf{k}'}\ . \tag{23}$$

To obtain Eq. (22), we have assumed that $P_{\mathbf{k}\mathbf{k}'}$ depends only on the angle between $\mathbf{k}$ and $\mathbf{k}'$, as is the case for elastic scattering by spherically symmetric impurity potentials. It follows that the impurity-scattering relaxation time τ_{imp} is independent of the $\mathbf{k}$ direction.

Performing the sum over $\mathbf{k}$ in Eq. (22) gives the Fiks-Huntington ballistic expression[38,39]

$$\mathbf{F}_w(\mathbf{r}_0)=-\frac{m\Omega\mathbf{J}(\mathbf{r}_0)}{e\tau_{\text{imp}}} \tag{24}$$

where $\mathbf{J}(\mathbf{r}_0)$ is the electron-charge current density incident upon the impurity. In the case of a bulk system, $\mathbf{J}(\mathbf{r}_0)=\mathbf{J}_0=\mathbf{E}_0/\rho_0$ and, ignoring small corrections associated with deviations from Mathiessen's rule, $\delta\rho=m/n_0e^2\tau_{\text{imp}}$. The wind-force expression (24) now becomes

$$\mathbf{F}_w|_{\text{bulk}}=-n_0e\Omega\delta\rho\mathbf{J}_0 \tag{25a}$$

$$=-n_0e\Omega\left[\frac{\delta\rho}{\rho_0}\right]\mathbf{E}_0\ . \tag{25b}$$

The volume factor Ω cancels in the final result because $\delta\rho\propto(\tau_{\text{imp}})^{-1}\propto\Omega^{-1}$.

The wind-force expressions (25) are more general than our derivation indicates. They hold, for example, in the case of isotropic impurity scattering in a thin film having specular surfaces if the background scattering process is uniform.[17] In fact, wind-force expressions similar to Eqs. (25) hold for the case of an arbitrary scattering potential (not necessarily spherically symmetric) immersed in a medium described by uniform background scattering. For this case, the generalization of Eq. (25b) is

$$\mathbf{F}_w|_{\text{bulk}}=-n_0e\Omega\frac{\delta\overleftrightarrow{\rho}\cdot\mathbf{E}_0}{\rho_0}\ , \tag{26}$$

where $\delta\overleftrightarrow{\rho}$ is the change in the resistivity tensor caused by the introduction of the impurity. Equation (26) applies to arbitrary "impurities" such as extended defects or impurity clusters provided that $\mathbf{F}_w$ is understood to refer to the net wind force on the defect or cluster. A derivation of Eq. (26) based upon the Boltzmann equation is given in the Appendix.

In obtaining Eqs. (25) and (26), we have implicitly ignored the renormalization of electron density, velocity, and density of states, as well as changes in the background scattering rate induced by the presence of a single impurity immersed in the electron gas. Such effects lead to corrections in $\mathbf{F}_w$ that are higher order in $(k_F l)^{-1}$, and therefore need not be considered in calculations of $\mathbf{F}_w$, but they are formally of the same order as $\mathbf{F}_d$. In this connection, we remark that in the literature[6,8,10] there are derivations of expressions for the *total* force $\mathbf{F}_w + \mathbf{F}_d$ which are identical to the expressions (25), which we have derived for the wind force only. These derivations are based upon momentum-balance arguments and appear to be quite general. It is not clear, however, that all relevant renormalization effects were incorporated in these papers. Specifically, impurity-induced changes in the background-scattering rate were neglected in the derivations. In any case, Eqs. (25) and (26) are valid expressions for the wind force to leading order in $(k_F l)$.

In the next section, we evaluate $\mathbf{F}_w$ and $\mathbf{F}_d$ for specific mesoscopic systems and investigate the connection between $\mathbf{F}_w$ and $\delta\rho$. The results which we shall obtain differ markedly from the results for bulk systems. This difference arises for two reasons: First, $g_{\mathbf{k}}$ is not equal to the corresponding bulk expression (1); and second, the field inhomogeneities are so great that the average macroscopic field is not representative of the external field, $\mathbf{E}_0(\mathbf{r}_0)$, acting on the impurity.

III. APPLICATION TO MESOSCOPIC SYSTEMS

A. One-dimensional disordered conductors

Consider a one-dimensional chain of potentials v_i representing a sequence of impurities in a one-dimensional system at zero temperature. The total potential has the form

$$V(z) = \sum_i v_i(z - z_i) \ , \tag{27}$$

where z_i is the position of the ith impurity. We shall take the impurity potentials to be localized and nonoverlapping so that $V=0$ regions exist between impurities.

We consider the Landauer configuration,[28,29] where reservoirs acting as sources and sinks of electrons are attached to the ends of the chain. The length of the chain is L, and we assume that $L \ll l$, where l is the mean free path for background scattering and other inelastic processes. We can therefore totally neglect all scattering processes other than the elastic electron-impurity scattering due to $V(x)$. This greatly simplifies the conductivity and electromigration problems.

Let the chemical potentials of the reservoirs be μ_1 and μ_2 on the left- and right-hand ends of the chain, respectively. Since we are concerned with linear response, we take $\Delta\mu \equiv \mu_1 - \mu_2$ to be arbitrarily small and positive. The reservoirs give rise to an incident distribution of electrons g_k where for each electron spin

$$g_k = \Delta\mu\Theta(k)\delta(\varepsilon_k - \varepsilon_F) \ , \tag{28}$$

where $\Theta(k)$ is the unit step function, i.e., $\Theta(k)=1$ for $k \geq 0$ and equals zero for $k<0$. A positive (negative) value of k refers to electrons travelling to the right (left). The incident electrons in g_k are reflected or transmitted by the impurity chain, with probabilities R and T, respectively.

Calculation of the potential drop across the chain, using the one-dimensional forms of Eqs. (3) and (5) gives for the left- minus right-potential difference

$$\delta\Phi_L - \delta\Phi_R = -\Delta\mu R/e \ , \tag{29}$$

where we used the one-dimensional density of states $dn/dE = 2/\pi\hbar v_F$, including both spins. To obtain Eq. (29), we evaluated $\delta n_w(z)$ as an average of expression (3) over a window a few wavelengths in width. The effect of this is to eliminate cross terms in $\delta n_w(z)$ due to the $\exp(\pm ikz)$ components of $\psi_k^{(+)}(z)$. This procedure is justified in the conductivity problem, where we are interested in a local average field, i.e., we want the persistent part of $\delta\Phi(\mathbf{r})$ and not the Friedel oscillations. This procedure is also consistent with the use of Eq. (5) rather than Eq. (4).

The net transmitted particle current j_t is given by

$$j_t = \frac{1}{L}\sum_k g_k v_k T = \frac{\Delta\mu}{\pi\hbar} T \ . \tag{30}$$

The resistivity ρ of the chain equals the average field divided by the charge current, i.e.,

$$\rho = \frac{-(\delta\Phi_L - \delta\Phi_R)/L}{-e j_t} \ , \tag{31}$$

which, after substitution of expressions (29) and (30), gives the celebrated Landauer formula[28]

$$\rho = \frac{\pi\hbar}{Le^2}\frac{R}{T} \ . \tag{32}$$

The Landauer formula is appropriate when the voltage probes measure the self-consistent potential $\delta\Phi(z)$ across the sample.[19,20] In the experimental configurations thus far achieved, this is apparently not the case. Rather, it has been argued[19–22] that in a standard two-probe measurement between voltage pads, the relevant quantity is the chemical potential difference $\Delta\mu$ of the pads and not the electrostatic potential difference across the disordered region. In this case, the new resistivity ρ', which includes the contact resistances at the conductor-reservoir interfaces, is given by[19–22]

$$\rho' = \frac{-(\Delta\mu/e)/L}{-e j_t} = \frac{\pi\hbar}{Le^2}\left[\frac{1}{T}\right] \ . \tag{33}$$

Now consider the electromigration force F^i on the ith impurity in the chain, which we write as the sum of direct and wind forces, i.e., $F^i = F_d^i + F_w^i$. According to our discussion after Eq. (21) it follows that the external field $E_0(z_i)$ vanishes. Consequently, by Eq. (21),

$$F_d^i = 0 \ . \tag{34}$$

The vanishing of the direct force means that the impurity senses only the wind force. The latter is now evaluated from the momentum flux on the ith impurity. Consider an electron incident onto the chain in state k, and let $a_L^+(k)$ and $a_L^-(k)$ be the plane-wave amplitudes for the electron scattering state immediately to the left of the impurity. Specifically, a_L^+ and a_L^- are the coefficients of the $\exp(ikz)$ and $\exp(-ikz)$ components, respectively, of $\psi_k^{(+)}(z)$. Similarly, define $a_R^+(k)$ and $a_R^-(k)$ just to the right of the impurity. For a given incident k, the momentum/sec transferred to the impurity is found by calculating the product of the number of electrons/sec incident onto the impurity and the momentum carried per electron. The result is then summed over L,R, and $+,-$, taking into account direction of momentum flux. Finally a sum over k is performed. The result is

$$F_w^i = \sum_k g_k m v_k^2 [\,|a_L^+(k)|^2 + |a_L^-(k)|^2 - |a_R^+(k)|^2 - |a_R^-(k)|^2\,] \; . \tag{35}$$

Expression (35) can also be obtained from Eq. (18), rather than by the present momentum-transfer analysis.[39]

The wind force F_w^i bears no direct relationship to the additional resistivity due to the ith impurity. However, the total force on the impurities is related to the total resistivity. To see this, use the global form of Eq. (35) for the entire system, in which case, the factor in parentheses in Eq. (35) equals $2R/L$, and we obtain

$$F_w^{\text{tot}} = \frac{2k_F \Delta\mu R}{\pi} \; , \tag{36}$$

where $F_w^{\text{tot}} = \sum_i F_w^i$.

Upon comparing Eqs. (29) and (36) we deduce that

$$F_w^{\text{tot}} = -\frac{2ek_F}{\pi}(\delta\Phi_L - \delta\Phi_R) \; . \tag{37}$$

Thus, the total electromigration driving force directly measures the self-consistent potential drop across the conductor. We can recast Eq. (37) in terms of the Landauer resistivity (32). By inspection, we have

$$F_w^{\text{tot}} = -n_0 e L \rho J_0 \; , \tag{38}$$

where $n_0 = 2k_F/\pi$ is the equilibrium 1D carrier density and $J_0 = -ej_t$ is the charge current. Note the striking similarity between Eq. (38) and the result (25a) for a bulk system. In the case of a single impurity between reservoirs, F_w^{tot} is the wind force on the impurity, and ρ becomes the additional resistivity due to that impurity. Then Eq. (38) becomes the 1D form of Eq. (25a), despite the fact that Eq. (25a) refers to a bulk system dominated by background scattering.

B. Impurity layer between reservoirs

We now consider the mesoscopic system consisting of a layer of impurities sandwiched between two reservoirs. The impurity layer is modeled within a jellium picture as a uniform slab bounded by the surfaces $z = \pm d/2$. This model can also be applied to the description of a grain boundary within a jellium picture.[40] Admittedly, the model is rather crude in that it neglects the discrete structure of the impurity atoms (or the grain boundary, in the second application). Nonetheless, it offers some valuable insights into the conduction-electromigration problem.

The Landauer configuration of Sec. III A is again assumed, with the reservoirs having chemical potential μ_1 and μ_2 lying at $z < L/2$ and $z > L/2$, respectively. As before, L is much less than the mean free path due to background scatterers. In previous work on the conductivity of such systems[25] a multichannel Landauer formula[23] was employed. Here we approach the problem more directly, by means of the general framework described in Sec. II and Sec. III A. The major difference between the present system and that of Sec. III A is the three-dimensional nature of the distribution of electrons emitted by the reservoirs. In place of Eq. (28), we now have

$$g_{\mathbf{k}} = \Delta\mu\,\Theta(k_z)\,\delta(\varepsilon_k - \varepsilon_F) \; . \tag{39}$$

Since the scattering potential in the system is independent of x and y, and vanishes for $|z| > d/2$, the scattering properties can be specified in terms of reflection and transmission coefficients, $R(\theta)$ and $T(\theta)$, respectively, where $\theta = \cos^{-1}(k_z/k_F)$ is the angle of incidence, and $R(\theta) + T(\theta) = 1$. For $k_z > 0$, the scattering states outside the impurity layer have the form

$$\begin{aligned}\psi_{\mathbf{k}}^{(+)}(\mathbf{r}) &= \frac{1}{\Omega^{1/2}}[e^{i\mathbf{k}\cdot\mathbf{r}} + r(\theta)e^{i\mathbf{k}^*\cdot\mathbf{r}}] \quad \left[z < -\frac{d}{2} \right] \\ &= \frac{1}{\Omega^{1/2}} t(\theta) e^{i\mathbf{k}\cdot\mathbf{r}} \quad \left[z > \frac{d}{2} \right] \; ,\end{aligned} \tag{40}$$

where $|r(\theta)|^2 = R(\theta)$, $|t(\theta)|^2 = T(\theta)$, and $\mathbf{k}^* = (k_x, k_y, -k_z)$. For $k_z < 0$, the two forms in Eq. (40) switch domains.

The potential drop across the impurity slab can be found from Eqs. (3), (5), (39), and (40). Again, as discussed in connection with Eq. (29), we discard the Friedel-oscillation terms in $|\psi_{\mathbf{k}}^{(+)}(\mathbf{r})|^2$, and obtain

$$\delta\Phi_L - \delta\Phi_R = -\frac{\Delta\mu}{e}\int_0^1 d\cos\theta\, R(\theta) \; . \tag{41}$$

The net transmitted particle current density $\mathbf{j}_t$ is given by

$$\begin{aligned}\mathbf{j}_t &= \frac{1}{\Omega}\sum_{\mathbf{k}} g_{\mathbf{k}} \mathbf{v}_{\mathbf{k}} T(\theta) \\ &= \hat{z}\frac{\Delta\mu k_F^2}{2\pi^2\hbar}\int_0^1 d\cos\theta \cos\theta\, T(\theta) \; .\end{aligned} \tag{42}$$

The resistivity ρ due to the impurity slab is found from Eqs. (31), (41), and (42). The resulting generalization of the Landauer formula (32) is

$$\rho = \frac{2\pi^2\hbar}{Le^2k_F^2} \frac{\int_0^1 d\cos\theta\, R(\theta)}{\int_0^1 d\cos\theta\cos\theta\, T(\theta)} \; . \tag{43}$$

The resistivity corresponding to expression (33), with the voltage reckoned with respect to the chemical-potential difference of the reservoirs, is

$$\rho' = \frac{2\pi^2\hbar}{Le^2k_F^2} \frac{1}{\int_0^1 d\cos\theta\cos\theta\, T(\theta)} \; . \tag{44}$$

We now consider the net electromigration force on the impurity layer. Although electromigration of the layer involves the motion of individual atoms within the layer, we treat the layer as a single impurity entity. From the discussion following Eq. (21), it follows that the external field at the layer vanishes. Consequently, we again find

$$\mathbf{F}_d = 0 \ .$$

The net wind force on the layer can be calculated from Eq. (20), using the explicit form of $P_{\mathbf{k}\mathbf{k}'}$ for the layer, namely,

$$P_{\mathbf{k}\mathbf{k}'} = \frac{A}{\Omega} v_F \cos\theta [R(\theta)\delta_{\mathbf{k}',\mathbf{k}^*} + T(\theta)\delta_{\mathbf{k}'\mathbf{k}}] \ , \tag{45}$$

where A is the area of the impurity layer. This leads to

$$\mathbf{F}_w = \hat{z}\frac{A k_F^3 \Delta\mu}{\pi^2}\int_0^1 d\cos\theta \cos^2\theta R(\theta) \ . \tag{46}$$

Because of the different $\cos\theta$ weight factors in the integrands of expressions (41) and (46), there is no longer any direct connection between $\mathbf{F}_w$ and $\delta\Phi_L - \delta\Phi_R$. Contrary to the results for the bulk and 1D systems, i.e., Eqs. (25a) and (38), respectively, $\mathbf{F}_w$ is not proportional to the product of $\mathbf{J}_0$ and the impurity resistivity.

We now turn to the problem of an impurity layer in a bulk system which is dominated by uniform background scattering. Using expression (1) for $g_{\mathbf{k}}$, we find that for this case, Eqs. (41) and (46) are replaced by

$$\delta\Phi_L - \delta\Phi_R = -2\tau v_F E_0 \int_0^1 d\cos\theta \cos\theta R(\theta) \tag{47a}$$

and

$$F_w = \hat{z}\frac{2 A k_F^3 e \tau v_F E_0}{\pi^2}\int_0^1 d\cos\theta \cos^3\theta R(\theta) \ , \tag{47b}$$

respectively, where we have chosen $\mathbf{E}_0$ along the negative z direction. The voltage drop (47a) occurs in the immediate vicinity of the impurity layer (within an electron screening length). Recently, Kirtley, Washburn, and Brady[41] have made scanning-tunneling-microscope (STM) measurements across a grain boundary in a current-carrying film. From their measurements they deduce that the local potential $\delta\Phi(\mathbf{r})$ does drop in the immediate vicinity of a grain boundary. Such behavior in $\delta\Phi(\mathbf{r})$ is consistent with our analysis and with earlier work by Landauer.[1,20,21,29] We caution, however, that it has yet to be demonstrated that STM measurements provide a direct measurement of $\delta\Phi(\mathbf{r})$.[42]

An interesting feature of the problem of a smooth impurity layer in bulk is that the extra voltage caused by the introduction of the layer is not totally localized at the layer. There is an additional voltage which is caused by the injection of the scattered electrons from the layer into the resistive background medium. The corresponding additional potential builds up over a length scale on the order of a mean free path, l, on either side of the layer. In the terminology of residual resistivity dipoles,[1,16] the close-in dipole has a different strength than the far-field dipole. A similar result was obtained for an impurity in a thin film.[17] Following the analysis of Ref. 17, it is easy to show that the total far-field potential drop across the barrier is given by

$$(\delta\Phi_L - \delta\Phi_R)_{\text{tot}} = -6\tau v_F E_0 \int_0^1 d\cos\theta \cos^3\theta R(\theta) \ . \tag{47c}$$

The close-in potential drop (47a) is essentially complete within an electron screening length of the layer, while the asymptotic drop (47c) is essentially complete within a mean free path of the layer. Superimposed on this local potential field is the linear potential $-\mathbf{r}\cdot\mathbf{E}_0$ due to the uniform background field. The extra resistance due to the impurity layer arises from the extra potential drop (47c) measured across the sample. For the case of weak scattering [$R(\theta) \ll 1$], the Boltzmann equation analysis of the Appendix applies. We would therefore expect that the extra resistivity arising from the layer is related to the wind force [Eq. (47b)] according to Eq. (26). This expectation is readily verifiable from Eqs. (47b) and (47c). We emphasize that the resistivity of a bulk system containing a weakly-scattering impurity layer is not equal to the sum of the background resistivity and the Landauer resistivity associated with the *close-in* voltage drop, Eq. (47a). This Landauer resistivity is given by expression (43) with an additional factor of $\cos\theta$ appearing in the integrands due to the bulk form of g_k appropriate to this system. The lack of additivity of close-in Landauer resistivity and background resistivity is contrary to the result for one-dimensional systems.[24]

If we were to consider an atomistic model for an impurity layer, rather than a smooth barrier-potential model, the potential would be quite different. In a simple model consisting of dilute scatterers randomly distributed within a layer, we ignore multiple scattering within the layer. The resulting $\delta\Phi(\mathbf{r})$ equals the sum of dipole fields of the form (6) centered at each impurity. The random arrangement produces an average field which is characteristic of a localized dipole sheet. However, unlike the case for the smooth-layer model, there is no crossover to another value of the potential at distances on the order of a mean free path from the layer. (The close-in and far-field dipole strengths are identical.) For a physical impurity layer or grain boundary we would expect both specular and atomistic scattering features to be present. The specular, or smooth-layer model, is most applicable to ordered impurity layers; the atomistic model is most applicable to very disordered layers.

C. Impurity near a point contact

Consider the standard theoretical model of a point contact[43–46] as a circular aperture, of radius a, on an opaque plane, $z=0$, which separates two halves of an electron gas. A negative potential difference $-\Phi_0$, is applied across the contact from the left-hand side ($z<0$) to the right-hand side ($z>0$). This raises the Fermi level of the electron gas on the left-hand side by an amount $\Delta\mu = e\Phi_0$ with respect to the Fermi level on the right-hand side, thereby causing a net flow of electrons through the aperture, from left to right. The spreading of electrons as they emerge from the aperture gives rise to local variations in the electron density, current, and potential.

The aperture acts as a bottleneck to electron flow, and gives rise to the so-called "spreading resistance" or Sharvin resistance[47] for a point contact, namely

$$R_{\mathrm{Sharvin}} = \frac{4\pi\hbar}{e^2 k_F^2 a^2} \ . \tag{48}$$

Equation (48) holds in the regime where background scattering is negligible and the aperture diameter is substantially greater than an electron wavelength, so that wave-diffraction effects at the aperture can be neglected. We shall also restrict our analysis to this regime. By neglecting quantum-mechanical diffraction and interference effects, we shall be excluding from our considerations the recently observed phenomenon of conductance quantization at point contacts.[48] Such effects are contained in our approach through the presence of the exact scattering wave functions $\psi_{\mathbf{k}}^{(+)}(\mathbf{r})$ in expression (3) for $\delta n_w(\mathbf{r})$. Calculation of these wave functions for small apertures is a difficult task, and will be considered in a future study.[49] Here we restrict attention to the case of apertures much larger than the electron wavelength, so that the waves incident upon an impurity near the axis of the aperture can be approximated by plane waves.

To apply the method of Sec. II, we need the electron distribution function. For definiteness, consider a point $\mathbf{r}$ in the $z>0$ region. There is an excess distribution of electrons at this point $g_{\mathbf{k}}(\mathbf{r})$ over and beyond the equilibrium distribution that would exist in the $z>0$ region if no aperture were present. The excess is due to the additional electrons from the $z<0$ region that can reach point $\mathbf{r}$ by propagating ballistically through the aperture. (Recall that we are in the regime where wave diffraction and background scattering are neglected.) Thus,

$$g_{\mathbf{k}}(\mathbf{r}) = \Delta\mu\,\delta(\varepsilon_k - \varepsilon_F) \quad \text{for } \mathbf{k}\in\Omega_0(\mathbf{r}) \ , \tag{49}$$

where $\Omega_0(\mathbf{r})$ is the solid angle defined by the sheaf of all straight-line trajectories emerging from the point $\mathbf{r}$ after having come through the aperture. [When $\mathbf{r}$ is on the axis of the aperture, $\Omega_0(\mathbf{r}) = 2\pi(1 - z/\sqrt{a^2+z^2})$.]

The unscreened local electron pileup due to $g_{\mathbf{k}}(\mathbf{r})$ is denoted by $\delta n_w^0(\mathbf{r})$, the superscript zero indicating that the perturbation is for the pure contact, without any impurity. Evidently,

$$\delta n_w^0(\mathbf{r}) = \frac{1}{\Omega}\sum_{\mathbf{k}} g_{\mathbf{k}}(\mathbf{r}) = \Delta\mu \frac{dn}{dE}\left[\frac{\Omega_0(\mathbf{r})}{4\pi}\right] . \tag{50}$$

The perturbed electrostatic potential due to $\delta n_w^0(\mathbf{r})$ is denoted by $\delta\Phi^0(\mathbf{r})$, and, from Eqs. (5) and (50), we have

$$\delta\Phi^0(\mathbf{r}) = -\frac{\Delta\mu}{e}\left[\frac{\Omega_0(\mathbf{r})}{4\pi}\right] . \tag{51}$$

Since expression (51) represents the excess potential over the background averaged potential in the $z>0$ region, the total potential for $z>0$ is obtained by adding to expression (51) the applied potential, which we choose to have the odd-parity form, namely $\frac{1}{2}\Phi_0\mathrm{sgn}(z)$. Thus we rederive the standard result[43,46]

$$\delta\Phi_{\mathrm{tot}}^0(\mathbf{r}) = \frac{\Delta\mu}{2e}\left[1 - \frac{\Omega_0(\mathbf{r})}{2\pi}\right] , \tag{52}$$

where $\delta\Phi_{\mathrm{tot}}^0$ is the total self-consistent potential for $z>0$. The $z<0$ potential follows from the symmetry relation $\delta\Phi^0(-\mathbf{r}) = -\delta\Phi^0(\mathbf{r})$.

The local charge-current density at point $\mathbf{r}$ is given by

$$\mathbf{J}(\mathbf{r}) = -\frac{e}{\Omega}\sum_{\mathbf{k}} g_{\mathbf{k}}(\mathbf{r})\mathbf{v}_{\mathbf{k}} \ , \tag{53}$$

which yields, after substitution of expression (49), the result

$$\mathbf{J}(\mathbf{r}) = -\frac{e\Delta\mu k_F^2}{4\pi^3\hbar}\int_{\mathbf{k}\in\Omega_0(\mathbf{r})} d\Omega_{\mathbf{k}}\hat{k} \ . \tag{54}$$

Evaluation of the net charge current I through the aperture using Eq. (54) gives $I = e\Delta\mu a^2 k_F^2/4\pi\hbar$. The Sharvin resistance (48) immediately follows from $R = \Phi_0/I$.

We now consider the effects of an impurity at position $\mathbf{r}_0$ near the point contact. The two quantities of experimental interest are the resistivity change δR and the electromigration force $\mathbf{F}$.

To determine δR we need to find the change in the electron charge current δI caused by the impurity. δI is due to those electrons in the distribution $g_{\mathbf{k}}(\mathbf{r}_0)$ that are backscattered through the aperture. Using the convention that δI is positive if it is in the same direction as the original current I, we find

$$\delta I = -e \sum_{\substack{\mathbf{k}\mathbf{k}' \\ \mathbf{k}'\in\Omega_0^*(\mathbf{r}_0)}} g_{\mathbf{k}}(\mathbf{r}_0) P_{\mathbf{k}\mathbf{k}'} \ , \tag{55}$$

where $\Omega_0^*(\mathbf{r}_0) = \Omega_0(-\mathbf{r}_0)$ is the solid angle subtended by the aperture when viewed from the impurity at $\mathbf{r}_0$. Thus only final states $\mathbf{k}'$ headed in the direction of the aperture are included in Eq. (55). Using the explicit form of $P_{\mathbf{k}\mathbf{k}'}$ in terms of the T matrix for impurity scattering, namely:

$$P_{\mathbf{k}\mathbf{k}'} = \frac{2\pi}{\hbar}|\langle\mathbf{k}'|T|\mathbf{k}\rangle|^2\delta(\varepsilon_k - \varepsilon_{k'}) \ , \tag{56}$$

we can write Eq. (22) in the form

$$\delta I = -\frac{e\Delta\mu\Omega^2}{16\pi^5\hbar^3 v_F^2}\int_{\mathbf{k}\in\Omega_0(\mathbf{r}_0)} dS_{\mathbf{k}} \int_{\mathbf{k}'\in\Omega_0^*(\mathbf{r}_0)} dS_{\mathbf{k}'}|T_{\mathbf{k}\mathbf{k}'}|^2 \ , \tag{57}$$

where the integrations are on the Fermi surface ($|\mathbf{k}| = |\mathbf{k}'| = k_F$). The impurity causes the point-contact resistance to increase by the amount

$$\delta R = -(\delta I/\Phi_0)R_{\mathrm{Sharvin}}^2 \ . \tag{58}$$

The electromigration force on the impurity contains the direct-force contribution of Eq. (21), namely:

$$\mathbf{F}_d = Z_d e[-\nabla\delta\Phi_{\mathrm{tot}}(\mathbf{r})]_{\mathbf{r}=\mathbf{r}_0} \ . \tag{59}$$

Since Eq. (52) implies that the potential drop $-\Phi_0$ occurs over a distance on the order of 2a across the aperture, the direct force is on the order of

$$\mathbf{F}_d \simeq -Z_d e\left[\frac{\Phi_0}{2a}\right]\hat{z} \tag{60}$$

for an impurity within a distance on the order of a from the aperture.

The wind force on the impurity follows from momentum transfer expression (20), which leads to

$$\mathbf{F}_w(\mathbf{r}_0)=\frac{\Delta\mu\Omega^2}{16\pi^5\hbar^3 v_F^2}\times\int_{\mathbf{k}\in\Omega_0(\mathbf{r}_0)} dS_{\mathbf{k}}\int dS_{\mathbf{k}'}|T_{\mathbf{k}\mathbf{k}'}|^2(\mathbf{k}-\mathbf{k}')\ , \tag{61}$$

where the surface integrals are on the Fermi surface. Note that electron scattering to all final states $\mathbf{k}'$ contributes to $\mathbf{F}_w$, whereas, according to Eq. (57), only the scattered electrons heading back toward the aperture contribute to δI. Consequently, $|\delta I|$ decreases more rapidly than F_w as the impurity moves away from the aperture. In particular, we find that for isotropic scattering ($T_{\mathbf{k}\mathbf{k}'}=\text{const}$) by an impurity at position z_0 on the axis of the aperture, Eqs. (57) and (61) imply that

$$\frac{F_w(z_0)}{\delta I}=-\frac{k_F}{e}\left[\frac{\sin^2\theta_0}{(1-\cos\theta_0)^2}\right], \tag{62}$$

where $\theta_0=\cos^{-1}[z_0/(a^2+z_0^2)^{1/2}]$ is the half-angle subtended by the aperture. Thus for $z_0 \gg a$, $F_w(z_0)/|\delta I|$ increases as $(z_0/a)^2$. We remark that for isotropic scatterers, F_w is proportional to δI even in the off-axis case.

The wind force can also be expressed in terms of the local current density $\mathbf{J}(\mathbf{r}_0)$ incident upon the impurity. The derivation leading to Eq. (24) also holds for the point-contact system. Thus,

$$\mathbf{F}_w(\mathbf{r}_0)=-\frac{-m\Omega\mathbf{J}(\mathbf{r}_0)}{e(\tau_{\text{imp}})_{\text{bulk}}}\ , \tag{63}$$

where J is given Eq. (54) and $(\tau_{\text{imp}})_{\text{bulk}}$ is the relaxation time for impurity scattering in bulk, and is given by Eq. (23).

Equation (63) shows that the wind-force scales with current density just as for the bulk system. When an impurity is very near the aperture, therefore, the actual current density at the aperture is the relevant quantity, and we can estimate the wind force as

$$F_w\simeq K\left[\frac{I}{\pi a^2}\right], \tag{64}$$

where $K\equiv F_w|_{\text{bulk}}/J_{\text{bulk}}$. The approximation (64) is excellent for an impurity in the aperture ($z=0$).

Because of the huge current densities that can be supported at a point contact, the wind force can be several orders of magnitude greater than in the bulk case. For a small aperture, the direct force is even more greatly enhanced with respect to bulk values because the external electric field E_0 at the aperture is proportional to current density and inversely proportional to a. Using Eqs. (60) and (64), we can estimate the relative importance of these forces. We find

$$\frac{F_d}{F_w}\simeq-\frac{Z_d e}{K}\left[\frac{2\pi^2\hbar}{e^3k_F^2 a}\right], \tag{65}$$

where we have used $\Phi_0=IR_{\text{Sharvin}}$ and expression (48). Note that, in principle, $|F_d|>F_w$ is possible when a is sufficiently small (provided that $k_Fa \gg 1$ so as not to contradict our neglect of diffraction at the aperture). Using $Z_d=Z$ and the calculated value of K for aluminum from Ref. 5, we find that Eq. (65) gives $F_d\simeq-\frac{1}{2}F_w$ for self-electromigration in aluminum when $a\simeq 14$ Å. This is in marked contrast to the case of bulk free-electronlike metals where

$$\left.\frac{F_d}{F_w}\right|_{\text{bulk}}=-\frac{Z_d e\rho_0}{K}\ . \tag{66}$$

Evaluation of this expression using values appropriate to nearly-free-electron conductors yields $|F_d|$ values which are typically much smaller than F_w values even at high temperature.

IV. DISCUSSION

Calculation of electrical conductivity and electromigration forces in mesoscopic systems is tractable within the common framework of the local-field method, which derives from basic ideas contained in Landauer's 1957 paper,[1] and which is described in Sec. II. The problem is simplified considerably for the mesoscopic systems considered in Sec. III because of the absence of background scattering and the choice of the Landauer reservoir configuration.[28,29] For such systems, the basic expressions of Sec. II are, in retrospect, relatively transparent. In particular, one need not resort to Kubo formulas, density matrices, etc., to establish them. Of course, the evaluation of the direct-field quantity Z_d [or in general $\delta n_d(\mathbf{r})$] does require more sophisticated approaches than discussed here; these have been given elsewhere.[14,33]

In this paper we have delved further into the self-consistent-screening aspects of the conductivity/electromigration problem and have shown that under an approximation on the screening-response kernel K in Eq. (4), one can establish the very useful force expressions (18) and (19). We remark that the treatment of self-consistent screening based on Eq. (5) is equivalent to the approach used in multichannel theories,[23] where the potential is deduced from the local chemical potentials for incoming and outgoing channels. Equation (4) is more rigorous, however, and it yields the true local potential field including Friedel oscillations and the effects of local inhomogeneities to all orders in the impurity potential.

The relationship (26) between the wind force and the resistivity change for arbitrary scattering complexes immersed in a bulklike medium is a generalization of expression (25a). The derivation in the Appendix makes it clear that the validity of Eq. (26) hinges upon the dominance of uniform background scattering, so that the bulk distribution function (1) can be taken as incident upon the scattering complex. If the background scattering processes were anisotropic, resulting in a $\mathbf{k}$-dependent relaxation time in Eq. (1), the connection between $\mathbf{F}_w$ and $\delta\overleftrightarrow{\rho}$ would be broken.

In mesoscopic systems there is, in general, no immediate connection between the electromigration force on an impurity and the resistivity change due to the impurity. However, for the 1D disordered conductor, the total electromigration force on the entire impurity chain is given by $F^{\text{tot}}=-n_0 eL\rho J_0$, according to Eq. (38). Thus, F^{tot} is a measure of the Landauer resistivity ρ rather than the resistivity ρ' of Eq. (33). On comparing Eqs. (29) and (36), we deduce that F^{tot} is a direct probe of the total self-consistent potential drop across the disordered region.

In the point-contact system, the wind force F_w, and the additional resistance δR due to an impurity in the system are both a measure of the impurity-scattering T matrix, as can be seen by comparing Eq. (61) with Eqs. (57) and (58). F_w and δR involve different weight factors over scattering direction, with δR being more sensitive than F_w to backscattering. However, for isotropic (s-wave) scatterers, F_w is proportional to δR, as can be seen from Eq. (61) and Eqs. (57) and (58).

In our treatment of the direct force we have been careful to define the external field $\mathbf{E}_0(\mathbf{r}_0)$ which appears in Eq. (21). In the general case of an impurity cluster of size much less than the background mean free path, $\mathbf{E}_0(\mathbf{r}_0)$ is the field which would exist at $\mathbf{r}_0$ in the absence of the impurity cluster. For the 1D disordered system of Sec. III A and the impurity-layer system of Sec. III B, there is no background scattering; the only scattering arises from the impurity cluster. Consequently, both $\mathbf{E}_0$ and δn_d vanish, and along with them, the direct force.

Our treatment of the direct field suggests a paradox. Consider a single impurity placed at $\mathbf{r}_0$ in a bulk medium where the background scattering is not truly uniform, but rather, arises from a random distribution of N_i impurities per unit volume. If one regards the system as a giant cluster of $N_i\Omega+1$ impurities, one is tempted to argue that even for this case, $\mathbf{E}_0(\mathbf{r}_0)$ vanishes and there is no direct force. In a technical sense, this is correct, but in this picture the resulting electron-wind problem is intractable, i.e., it would require solution of the quantum-mechanical multiple-scattering problem for $N_i\Omega+1$ impurities. It is more reasonable to employ the standard picture, which regards all other impurities as comprising a uniform-scattering background and which treats the scattering problem of a single impurity immersed in the background and exposed to $(g_{\mathbf{k}})_{\text{bulk}}$ of Eq. (1). From this viewpoint, $\mathbf{E}_0(\mathbf{r}_0)$ *does* exist, and the direct force is nonvanishing. To resolve the apparent paradox concerning the existence of $\mathbf{E}_0(\mathbf{r}_0)$, note that an electron-wind contribution corresponding to $\mathbf{E}_0(\mathbf{r}_0)$ is contained in the giant-cluster approach. $\mathbf{E}_0(\mathbf{r}_0)$ is effectively setup by the electron waves that are scattered by the background impurities, giving rise to dipole fields of the form (6) centered at each impurity. The volume average of these dipole fields is $\mathbf{E}_0(\mathbf{r}_0)$. Thus, for this example, depending on whether one considers background scattering in the usual macroscopic view, or in a (hopelessly) detailed microscopic view, the direct force does or does not exist. In the latter case, the direct force has been transformed into a wind-force contribution. This chameleonlike behavior of the direct force and wind force, along with their associated fields, is a fundamental aspect of electron transport in impurity-dominated bulk systems which has been unacknowledged in previous studies. An understanding of this point requires a local-field description of the system; it is totally missed in the conventional independent-particle picture, even if the Kubo formalism is invoked.

With regard to the discussion in Sec. I concerning the Kubo formalism versus the local-field method, we point out that an uncritical application of the Kubo linear-response theory based upon the existence of a uniform external field $\mathbf{E}_{\text{ext}}$ fails to give the correct local field in the case of the mesoscopic systems described in Sec. III A and III B. Within such a linear-response theory, the local field is obtained from Eq. (10) with $\mathbf{E}_0$ replaced by $\mathbf{E}_{\text{ext}}$. The result is

$$\begin{aligned}\mathbf{E}_L(\mathbf{r}_0)&=\mathbf{E}_{\text{ext}}-\int \delta n(\mathbf{r})\nabla_{\mathbf{r}_0}u(\mathbf{r})d^3r\\&=\mathbf{E}_{\text{ext}}-\lim_{\omega\to 0}\frac{\langle\langle \nabla_{\mathbf{r}_0}u;\mathbf{v}\rangle\rangle\cdot\mathbf{E}_{\text{ext}}}{i\omega}\,,\end{aligned}\tag{67}$$

where we have defined $u(\mathbf{r})=e/|\mathbf{r}-\mathbf{r}_0|$. In the second line, the double angular bracket denotes the usual Kubo correlation function, which results here from processing $\delta n(\mathbf{r})$ within Kubo formalism.[7,10,13] If we now identify $\mathbf{E}_{\text{ext}}$ to be the external field associated with the voltage drop $\Delta\mu/e$ between the reservoirs which are at the ends of our mesoscopic system, we would set $E_{\text{ext}}=\Delta\mu/eL$. The calculated local electric field of Eq. (67) now erroneously contains a uniform contribution from this $\mathbf{E}_{\text{ext}}$, leading to an erroneous direct force $Z_d e\mathbf{E}_{\text{ext}}$. In reality, for these systems there is no external field, and no direct force. In fact, for 1D mesoscopic systems, the local electric field between scatterers vanishes when averaged over a few wavelengths so as to wash out Friedel oscillations.

A number of points should be made concerning the possible use of electromigration as a practical probe of the local transport field in mesoscopic systems. First, the electromigration driving force measures the local field at the impurity in the presence of that impurity. Hence, electromigration is not an ideal, noninvasive probe of the pre-existing transport field. Second, there exists at least one other probe, namely, the STM, which can be applied to mesoscopic systems. This has been demonstrated by Kirtley, Washburn, Brady,[41] but further work is needed to establish the usefulness of the STM as a probe of the local transport field.[42] Third, low temperatures are required in studies of most mesoscopic systems to ensure that the inelastic mean free path is greater than the length of the sample. (The impurity layer and point-contact systems are exceptions.) At these low temperatures, atomic diffusion is extremely slow, and therefore, electromigration is extremely difficult to observe. Finally, electromigration experiments may be difficult to interpret. Inferring the strength of the electromigration driving force from the measured migration rates, and comparing with theory, requires some knowledge of the diffusion kinetics and structural inhomogeneities which influence them.

Despite the aforementioned difficulties in using electromigration as a practical probe of the local transport field, experimental studies of electromigration in mesoscopic systems would be interesting in their own right. Perhaps the most interesting of the mesoscopic systems, as far as electromigration experiments are concerned, is the point-contact system. Our analysis of Sec. III C shows that the wind force can be greatly enhanced in this system due to the very high current densities which can be made to flow through the contact. We also found that the direct force can be enhanced by an even greater amount when the contact radius, a, is sufficiently small. In the case of aluminum, the magnitude of the direct force is approximately 50% of the magnitude of the wind force when $a \approx 14$ Å. This suggests that point contacts may be an effective probe of the most controversial and fundamental aspect of electromigration theory, namely: the direct force. Recent experiments[50] suggest that electromigration through a point contact in a metallic microstructure has been observed.

Note Added. Equations (18) and (19) are more general than our derivation in Sec. II indicates, and, in fact, can be derived from Eqs. (16) and (17) without making any approximations to the kernel K or the screened potential V. [R. S. Sorbello (unpublished).]

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APPENDIX: DERIVATION OF EQ. (26)

The expression (26) relating wind force and impurity resistivity for a bulklike system can be derived from the Boltzmann equation

$$e\mathbf{v}_{\mathbf{k}}\cdot\mathbf{E}_0\delta(\varepsilon_k-\varepsilon_F)=-\sum_{\mathbf{k}'}(g_{\mathbf{k}}-g_{\mathbf{k}'})(P_{\mathbf{kk}'}+P^0_{\mathbf{kk}'})\ , \tag{A1}$$

where $P_{\mathbf{kk}'}$ is, as before, the transitional probability appropriate to a general scattering potential V, and $P^0_{\mathbf{kk}'}$ is the transitional probability for the background scattering, which is assumed to be isotropic (independent of the directions of $\mathbf{k}$ and $\mathbf{k}'$).

For a single impurity, or for an extremely dilute concentration of impurities, we can regard P to be much smaller than P_0. We can easily solve for $g_{\mathbf{k}}$ in this $P \ll P_0$ limit by writing $g_{\mathbf{k}}=g^0_{\mathbf{k}}+\delta g_{\mathbf{k}}$, where $g^0_{\mathbf{k}}$ is the solution appropriate to background scattering only, and $\delta g_{\mathbf{k}}$ is first order in P. We find that

$$\delta g_{\mathbf{k}}=-\tau\sum_{\mathbf{k}'}(g^0_{\mathbf{k}}-g^0_{\mathbf{k}'})P_{\mathbf{kk}'}\ , \tag{A2}$$

where $g^0_{\mathbf{k}}=-\tau e\mathbf{v}_{\mathbf{k}}\cdot\mathbf{E}_0\delta(\varepsilon_k-\varepsilon_F)$, and $\tau^{-1}=\sum_{\mathbf{k}'}P^0_{\mathbf{kk}'}$, which is the scattering rate associated with background scattering. $\delta g_{\mathbf{k}}$ gives rise to a current change $\delta\mathbf{J}$, where

$$\delta J_i=\frac{-e}{\Omega}\sum_{\mathbf{k}'}\delta g_{\mathbf{k}}(\mathbf{v}_{\mathbf{k}})_i\ . \tag{A3}$$

The corresponding change in the conductivity tensor $\overleftrightarrow{\sigma}$ is defined via

$$\delta J_i=\sum_j \delta\sigma_{ij}E_{0j}\ . \tag{A4}$$

Substitution of (A2) into (A3), and subsequent comparison with (A4) leads to

$$\delta\sigma_{ij}=-\frac{\tau^2e^2}{\Omega}\sum_{\mathbf{kk}'}(\mathbf{v}_{\mathbf{k}}-\mathbf{v}_{\mathbf{k}'})_j(\mathbf{v}_{\mathbf{k}})_iP_{\mathbf{kk}'}\delta(\varepsilon_k-\varepsilon_F)\ . \tag{A5}$$

Now the ith component of the wind force of Eq. (20) is

$$(\mathbf{F}_w)_i=\sum_j\sum_{\mathbf{kk}'}\hbar(\mathbf{k}-\mathbf{k}')_iP_{\mathbf{kk}'}[-\tau e(\mathbf{v}_k)_jE_{0j}\delta(\varepsilon_k-\varepsilon_F)]\ . \tag{A6}$$

Comparing (A5) and (A6), and using the Onsager symmetry relation $\delta\sigma_{ij}=\delta\sigma_{ji}$, we find

$$(\mathbf{F}_w)_i=n_0e\Omega\sum_j\left[\frac{\delta\sigma_{ij}}{\sigma_0}\right]E_{0j}\ , \tag{A7}$$

where $\sigma_0=n_0e^2\tau/m$. Since we are effectively assuming one impurity per unit volume, $\delta\sigma_{ij}\ll\sigma_0$, and we can then take $\delta\sigma_{ij}/\sigma_0=-\delta\rho_{ij}/\rho_0$ in (A7), thereby obtaining Eq. (26).

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[32] For arbitrary bare impurity potentials, all our equations remain valid except Eqs. (7)–(9). These are readily generalized, by writing the arbitrary bare potential in the form of expression (7) with $Z \rightarrow Z(\mathbf{r}_0)$ and subsequently integrating over $\mathbf{r}_0$. Thus $Z(\mathbf{r}_0)e$ would now represent the charge-density distribution of the ion core. The right-hand side of Eqs. (8) and (9) would then require the corresponding integral over $\mathbf{r}_0$.

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