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Incompleteness of the Landauer formula for electronic transport

Giovanni Vignale
Department of Physics, University of Missouri–Columbia, Columbia, Missouri 65211, USA

Massimiliano Di Ventra
University of California–San Diego, La Jolla, California 92093, USA

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We show that the Landauer formula for the conductance of a nanoscale system is incomplete because it does not take into account many-body effects which cannot be treated as contributions to the single-particle transmission probabilities. We show that the physical origin of these effects is related to the viscous nature of the electron liquid and we develop a perturbative formalism, based on the time-dependent current-density-functional theory, for calculating the corrections to the resistance in terms of the "Kohn-Sham current distribution" and the exchange-correlation kernel. The difficulties that still remain in calculating the latter are critically discussed.

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I. INTRODUCTION

The trend toward extreme miniaturization of electronic devices provides strong motivation for theoretical studies aimed at characterizing and understanding the electrical transport properties of quantum-mechanical systems.[1] Here, by "quantum system" we mean a molecular structure or cluster of atoms or perhaps a microscopic region defined on the surface of a semiconductor. Either way, this system is connected to an external circuit which maintains current flow via electron sources.

In the case of steady-state transport, this complicated nonequilibrium many-body problem is oftentimes simplified by *conceptually* replacing the electron sources with ideal reservoirs, whose role is to define a local electron distribution and a local electrochemical potential at which electrons are injected in or extracted from the system.[2–5] The reservoirs are conceptual constructs which allow us to map the transport problem onto an *ideal* stationary scattering one so that the time derivative of all local physical properties of the system and the current is zero.[6]

As a further simplification, one assumes that these reservoirs are adiabatically "connected" to leads in which noninteracting electrons are free to propagate before scattering at the lead-system interface.[3] The leads are only a convenient region of space where scattering states can be developed into an appropriate basis of the Hilbert space. This viewpoint to electrical conduction is known as Landauer approach.

A schematic of this approach applied to a system connected to several leads is shown in Fig. 1 where the shaded region represents the system and the white regions are the leads, numbered $1-N$. The contacts between the leads and the system can be very complicated and should be considered part of the system. The proper lead, far from the contact, is a single-electron wave guide, which we can assume to have constant electrochemical potential μ_i $(i=1,..,N)$. At equilibrium all the leads are at the same electrochemical potential μ and no current flows in or out of the system. As we move slightly away from equilibrium, the currents flowing in the leads will be related to the electrochemical potentials by the linear relationships

$$I_i = \sum_{j=1}^{N} G_{ij}\mu_j, \tag{1}$$

where the currents I_i are reckoned positive when they flow out of the system and negative when they flow into the system. The coefficients G_{ij} are the linear conductances of the system. In an ideal steady-state situation (μ_i and I_i independent of time) the conservation of charge implies that the sum of all the currents is zero and therefore (for every terminal j)

$$\sum_{i=1}^{N} G_{ij} = 0. \tag{2}$$

Furthermore, the condition that the currents vanish when all the chemical potentials are equal implies that

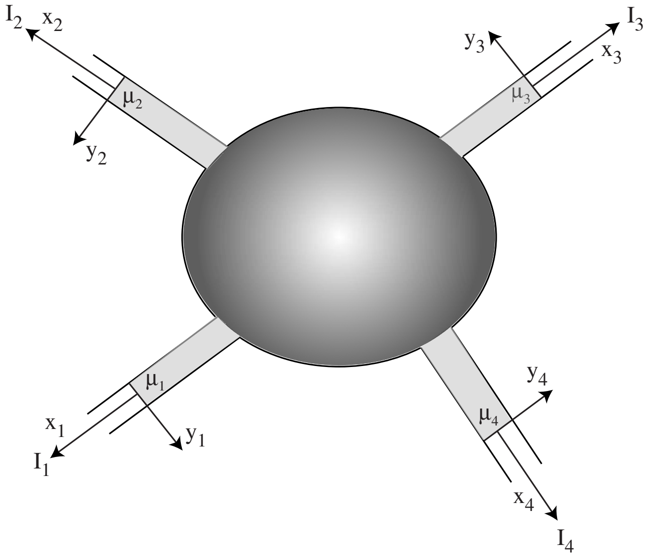

FIG. 1. Schematic of a quantum system in a multiterminal configuration. The central region is connected to leads of noninteracting electrons, in turn connected adiabatically to reservoirs of electrons.

$$\sum_{j=1}^{N} G_{ij} = 0. \tag{3}$$

It follows that the off-diagonal conductances G_{ij}, with $i \neq j$, are sufficient to completely characterize the linear steady-state response of the system.

The Landauer formula offers an appealing way to relate G_{ij} to the quantum-mechanical properties of the system. In this theory G_{ij} is proportional to the quantum-mechanical probability that a single electron coming from lead i with energy E be transmitted into a different lead j at the same energy. In linear response and at zero temperature, this energy can be taken to be the Fermi energy E_F of the system. We call this coefficient $T_{ij}(E_F)$ and notice that, in general, it is a sum of all the partial probabilities of transmission from one of the momentum states of the incoming electron at energy E_F to one of the momentum states of the outgoing electron at the same energy (see, e.g., Refs. 1 and 5). Thus, the Landauer formula reads

$$G_{ij} = \frac{2e^2}{h} T_{ij}(E_F), \quad (i \neq j). \tag{4}$$

It is important to note that the mathematical description of this approach relies on scattering theory, namely, on the transmission properties of single electrons in the leads that scatter at the leads-system interface. Therefore, for this description to be valid any interaction between electrons can only be included at a mean-field level. Many-body interactions beyond mean field destroy the concept of single-particle transmission probability and, in fact, when taken into account also in the leads, they do not even allow for the derivation of a closed form for the total current.[1,7,8] All of the above issues are particularly relevant in nanoscale systems, where the current densities at the junction can be substantially larger than in the bulk. A large current density implies a large number of scattering events per unit time and unit volume, thus making the description of transport phenomena in terms of noninteracting particle properties questionable.[1]

It should thus not come as a surprise, and this is what we set to clearly show in this paper, that the Landauer formula (4) represents an incomplete description of electrical transport in nanoscale systems. This point is particularly relevant these days, since there has been a surge of theoretical activities aimed at calculating the transport properties of these systems from "first principles." A popular way to tackle this problem is to extract the transmission function appearing in Eq. (1) from the one-electron Green's function,[9] which is calculated from the self-consistent potential of the ground-state density-functional theory (DFT).[10] In this manner, one hopes to include the most important effects of the electron-electron interaction without losing the simplicity of the single-particle theory. Indeed, one expects that interactions control the positioning of the single-particle energy levels of the system with respect to the Fermi level and for this reason they have a large impact on the conductance.

However, from a more general theoretical standpoint things are not so simple. First of all, even if we assume that the physical approximations underlying the Landauer formula (1) are a reasonable starting point to describe electrical transport, the use of ground-state DFT in the present context is highly questionable, since one effectively uses a ground-state theory for an intrinsically nonequilibrium problem even in linear response and in the dc limit.[1,6]

Indeed—and this leads us to the central message of this paper—it is precisely the nonequilibrium nature of the transport problem which renders Eq. (4) untenable. In a practical realization of a transport experiment, electrons are in a state of nonequilibrium and, therefore, their correlations are time dependent even in the limit of zero frequency. These correlations give rise to scattering processes that *cannot* be described by a mean-field theory and, under certain conditions, may influence substantially their dynamics.

Therefore, the Landauer formula, which has been derived within a single-particle framework, cannot be uncritically transferred to the many-body context, hoping that a proper inclusion of many-body effects in the single-particle energy levels will always suffice. In fact, in this paper we show that there are many-body corrections to the Landauer formula, which *cannot* be formulated in terms of single-particle transmission probabilities.

In order to demonstrate this important point of principle we start from the rigorous formulation of the conductance in terms of the zero-frequency limit of the exact nonlocal conductivity tensor $\sigma_{ij}(\mathbf{r},\mathbf{r}';\omega)$ of the interacting many-electron system (ω is the frequency) in the linear-response regime. We then resort to the time-dependent current-density-functional theory (TDCDFT) (Refs. 11–13) to show that the conductivity tensor $\overleftrightarrow{\sigma}$ satisfies the integral equation

$$\overleftrightarrow{\sigma} = \overleftrightarrow{\sigma}_s - \overleftrightarrow{\sigma} \cdot \overleftrightarrow{\rho}_{\text{xc}} \cdot \overleftrightarrow{\sigma}_s \tag{5}$$

where $\overleftrightarrow{\sigma}_s$ is the resistivity tensor of a noninteracting system in the presence of a static potential V_s (also known as the Kohn-Sham potential) that reproduces the exact ground-state density and $\overleftrightarrow{\rho}_{\text{xc}}$ is a dynamical contribution that will be defined precisely in Sec. III.

The linear-response formulation of mesoscopic transport dates back to works by Fisher and Lee[14] and Baranger and Stone[15] in the 1980s and was recently combined with density-functional theory by several authors.[16–19] Because $\overleftrightarrow{\sigma}_s$ is the conductivity of a noninteracting system, it is possible to analyze it microscopically by the method of Fisher and Lee[14] (later generalized by Baranger and Stone[15]) and thus show that this part of the conductivity alone leads to the Landauer formula (1), with transmission probabilities computed from the Kohn-Sham potential V_s. This step is still within the assumptions of the Landauer approach, whereby the electron sources are replaced by conceptual reservoirs whose role is to populate the single-particle states according to different Fermi functions and these states can be developed in terms of the single-particle states of the leads. However, this is not the whole story, since there is also the contribution of the second term on the right-hand side of Eq. (5). In other words, within the Landauer viewpoint to conduction, even if we knew the *exact* Kohn-Sham potential, including all the self-interaction and nonlocal corrections which are responsible for the correct alignment of the one-electron energy levels, we would still be making an error in calculating the conductance from the Landauer formula (4).[20]

Next, we examine the nature of the correction to the Landauer formula. We observe that Eq. (5) is algebraically equivalent to the equation

$$\overleftrightarrow{\rho} = \overleftrightarrow{\rho}_s + \overleftrightarrow{\rho}_{\mathrm{xc}}, \tag{6}$$

where $\overleftrightarrow{\rho} \equiv \overleftrightarrow{\sigma}^{-1}$ is the exact nonlocal resistivity, $\overleftrightarrow{\rho}_s \equiv \overleftrightarrow{\sigma}_s^{-1}$ is the Kohn-Sham resistivity, and $\overleftrightarrow{\rho}_{\mathrm{xc}}$ is the contribution from many-body exchange and correlation. The resistivity controls the energy dissipation associated with a steady current distribution and the presence of the xc correction $\overleftrightarrow{\rho}_{\mathrm{xc}}$ implies that there are mechanisms of dissipation that are not taken into account in the Landauer approach of elastically scattering electrons, with relaxation and dephasing occurring only in the reservoirs.[21] What Eq. (6) tells us is that electron-electron interactions make up for additional dissipation within the system, a dissipation that is physically a manifestation of *electronic viscosity*. As a matter of fact, the simplest approximation for $\overleftrightarrow{\rho}_{\mathrm{xc}}$, which is derived from the Vignale-Kohn (VK) approximation to TDCDFT,[12] is expressed precisely in terms of the viscosity of a homogeneous electron liquid: this approximation shows that ρ_{xc} is a positive kernel, always giving rise to a positive contribution to dissipation (i.e., an increase in resistance).

The existence of viscosity contributions to the electrical resistance was first pointed out in Ref. 22, where these contributions were called *dynamical corrections* because, as we have discussed above and will show below, they vanish in a strictly ground-state formulation of the theory. However, the relation of such contributions to the Landauer formula had remained somewhat unclear (see also Ref. 16). The present work shows conclusively that the Landauer formula (4) is incomplete and the many-body corrections to it are precisely the "dynamical corrections" identified in Ref. 22.

The form of Eq. (6) suggests a simple perturbative approach to the calculation of the resistances R_{ij} (derived from the conductances G_{ij} and defined more precisely below) based on the minimal entropy-production principle of linear-response theory.[23] In brief, since the energy dissipation rate (proportional to the entropy production) computed from the single-particle (mean-field) theory is stationary with respect to a small variation of the Kohn-Sham current distribution $\mathbf{j}_s(\mathbf{r})$ (for given *total* currents in the leads) it follows that the additional dissipation due to the xc term is simply

$$W_{\mathrm{xc}} = \mathbf{j}_s \cdot \overleftrightarrow{\rho}_{\mathrm{xc}} \cdot \mathbf{j}_s \tag{7}$$

to first order in $\overleftrightarrow{\rho}_{\mathrm{xc}}$. From this formula, and from the knowledge of the Kohn-Sham current distribution, we can straightforwardly extract the xc contribution to the resistances. The formula for the xc two-probe resistance of a quantum point contact or molecular junction which we presented in Ref. 22 will be recovered as a special case of the general perturbative formulation.

Finally, we consider some quantitative aspects of the theory. It must be said that a compelling comparison between theory and experiments is still hampered in most cases by an imperfect characterization of the contact region. Keeping this in mind, it is now accepted that the theoretical calculations of the conductance of molecular junctions, using the Landauer approach and ground-state DFT, *overestimate* the measured conductance by at least an order of magnitude.[10] Part of this discrepancy can certainly be attributed to errors in determining the position of the energy levels of the system relative to the electrochemical potential in the leads—errors which in turn are intimately connected to self-interaction corrections, discontinuities in the xc potential as a function of particle number, and so on.[24] Even after correcting for these effects, however, it seems that the computed conductance remains larger than the observed one, and it is here that our many-body corrections can play a decisive role.

Our preliminary estimates of the size of the correction seem to indicate that the many-body viscous effects contribute only a small percentage to the total resistance.[22] For the case of two infinite jellium electrodes separated by a vacuum gap, the use of the viscosity as reported in Ref. 25 has shown an even smaller effect.[26] But this does not mean that the issue is settled.

First of all, it is important to note that these estimates have been based on an oversimplified description of the current density in nanoscale systems by neglecting transverse variations of both the density and current density.[22] For instance, as shown in Ref. 27 transverse density gradients increase the dynamical resistance. Quite generally, the transverse density and current-density gradients and the spatial variation of the viscosity must all be taken into account when evaluating the viscous resistance. This is particularly relevant in nanoscale systems where nonlinear (turbulent) effects have been recently predicted.[28–31] Therefore, for a given nanoscale system, these dynamical effects need to be evaluated with the self-consistent microscopic density and current-density distribution.

Aside from the above issues, there remains another and more fundamental source of uncertainty, namely, the value of the electronic viscosity which enters the dissipative kernel ρ_{xc}. In the concluding part of this paper we will argue that this value is still subject to a large uncertainty and we will outline the path along which better approximations might be obtained.

This paper is organized as follows. Section II reviews the general formulation for the conductance and the resistance of a nanoscale system in terms of nonlocal conductivity. In Sec. III we present the time-dependent current-density-functional approach to the calculation of the resistivity and demonstrate the existence of corrections to the Landauer formula (4). In Sec. IV we develop the perturbative approach to the calculation of the many-body corrections to the resistance. In Sec. V we illustrate the working of the formalism in a simple one-dimensional model, re-deriving and extending the informal estimates of Ref. 22. Finally, in Sec. VI we discuss the present difficulties in performing accurate calculations of the many-body corrections and outline a path toward more accurate estimates.

II. FORMULATION

Our starting point is the linear-response formula for the steady current density $\mathbf{j}$ in the presence of a steady electric field $\mathbf{E}$,

$$j_\alpha(\mathbf{r}) = \sum_\beta \int d\mathbf{r}' \sigma_{\alpha\beta}(\mathbf{r},\mathbf{r}')E_\beta(\mathbf{r}'), \tag{8}$$

where α and β denote cartesian indices and $\sigma_{\alpha\beta}(\mathbf{r},\mathbf{r}')$ is the real part of the conductivity tensor. The integral runs over the whole volume of the system depicted in Fig. 1 including the leads. The electric field, however, vanishes deep inside the leads. The above equation is satisfied for small electric fields of the form

$$\mathbf{E}(\mathbf{r}) = -\nabla_\mathbf{r}\phi(\mathbf{r}), \tag{9}$$

where $\phi(\mathbf{r})$ is an electrostatic potential of arbitrary shape, except for the constraint of tending to constant values

$$\phi(\mathbf{r}) \to \mu_i \tag{10}$$

deep into the ith lead.

Here, we assume that the electrostatic potential coincides with the electrochemical potential deep into the leads.[32] Because a steady current also satisfies the continuity equation

$$\nabla_\mathbf{r} \cdot \mathbf{j}(\mathbf{r}) = 0 \tag{11}$$

and because the current cannot be affected by a uniform shift of the electric potential in the whole space it follows that the conductivity tensor satisfies the conditions[15]

$$\sum_{\alpha\beta} \partial_\alpha \partial'_\beta \sigma_{\alpha\beta}(\mathbf{r},\mathbf{r}') = 0 \tag{12}$$

and

$$\sum_{\alpha\beta} \partial_\alpha \int_{C_j} dy'_j \sigma_{\alpha\beta}(\mathbf{r},\mathbf{r}')x_{j\beta} = 0, \tag{13}$$

where ∂_α is a short-hand notation for $\partial/\partial r_\alpha$ and ∂'_β stands for $\partial/\partial r'_\beta$; $\hat{x}_j$ is the outwardly directed unit vector in lead j and y_j is a short-hand notation for the coordinates perpendicular to $\hat{x}_j$, which are integrated over the cross section C_j of the jth lead (see Fig. 1 for a schematic).[33]

The current I_i in the ith lead is given by

$$I_i = \int_{C_i} dy_i \mathbf{j}(\mathbf{r}) \cdot \hat{x}_i = -\int_{C_i} dy_i \int d\mathbf{r}' \sum_{\alpha\beta} x_{i\alpha}\sigma_{\alpha\beta}(\mathbf{r},\mathbf{r}')\partial'_\beta \phi(\mathbf{r}'). \tag{14}$$

Following Baranger and Stone[15] we make use of Eqs. (10) and (12) and an integration by parts to find the intuitive result [cf. Eq. (1)]

$$I_i = \sum_{j=1}^N G_{ij}\mu_j, \tag{15}$$

where

$$G_{ij} = -\int_{C_i} dy_i \int_{C_j} dy'_j \sum_{\alpha\beta} x_{i\alpha}\sigma_{\alpha\beta}(\mathbf{r},\mathbf{r}')x_{j\beta}. \tag{16}$$

Note that up to this point we have made no approximation on the microscopic physical mechanisms that contribute to the conductance (16) apart from those embodied in the viewpoint represented in Fig. 1. Therefore, within this viewpoint, the conductance (16) contains, in principle, all many-body interactions even beyond mean field.

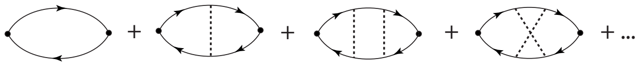

FIG. 2. Diagrams for the proper current-current response function. The solid dots represent (particle) current vertices. The solid lines represent fully dressed single-particle propagators and the dotted lines Coulomb scattering processes.

The next step is then to express the conductivity tensor in terms of a microscopic current-current response function. To this end we introduce the *proper* current-current response function, which yields the electric current response to the fully *screened* vector potential in the following manner:

$$j_\alpha(\mathbf{r},\omega) = -e^2 \sum_\beta \int d\mathbf{r}' \tilde{\chi}_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega)[A_\beta(\mathbf{r}') + A_{H,\beta}(\mathbf{r}')], \tag{17}$$

where $\mathbf{A}(\mathbf{r})$ is the external vector potential and $\mathbf{A}_H(\mathbf{r})$ is the vector potential additionally created by the screening charge.[34] The factor e^2 (e being the absolute value of the electron charge) is introduced to be consistent with the definitions used in other publications.[1,13,35] The use of the "proper" current-current response function as opposed to the "ordinary" one, which describes the response merely to the external vector potential, is required because we are seeking the current response to the physical electric field, which includes contributions from the induced space charge. Then the conductivity is

$$\sigma_{\alpha\beta}(\mathbf{r},\mathbf{r}') = -e^2 \lim_{\omega\to 0} \frac{\Im m \tilde{\chi}_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega)}{\omega}. \tag{18}$$

The proper current-current response function is best expressed in terms of an infinite series diagrams with two current vertices, such as the diagrams shown in Fig. 2 where the solid lines represent fully dressed particle propagators and dotted lines Coulomb interactions. Notice that this series does not contain any diagrams that can be divided into two parts by cutting a single Coulomb interaction line. It is the exclusion of these diagrams that makes our response function "proper" as opposed to "full."[34]

A. Mean-field approximation

In the special case of a noninteracting system, or a system interacting at a mean-field level, only the first term of the series survives and we get, following the standard rules,[35]

$$\sigma_{\alpha\beta}(\mathbf{r},\mathbf{r}') = -\pi e^2 \sum_{nm} \frac{\partial f(\epsilon_n)}{\partial \epsilon_n} W^{\alpha *}_{nm}(\mathbf{r}) W^\beta_{mn}(\mathbf{r}')\delta(\epsilon_n - \epsilon_m), \tag{19}$$

where n and m denote exact single-particle eigenstates with energies ϵ_n and wave functions $\psi_n(\mathbf{r})$, $f(\epsilon_n)$ is the Fermi distribution at the common chemical potential μ (before applying the bias) and temperature T, and $W^\alpha_{nm}(\mathbf{r})$ is the matrix element of the α component of the (particle) current operator between states m and n:

$$W_{nm}^{\alpha}(\mathbf{r}) = -\frac{i\hbar}{m}\{\psi_n^*(\mathbf{r})\partial_\alpha\psi_m(\mathbf{r}) - [\partial_\alpha\psi_n^*(\mathbf{r})]\psi_m(\mathbf{r})\}. \quad (20)$$

Equation (19) leads upon substitution in Eq. (16) to the standard Landauer formula (4).[14,15] The calculation is quite subtle, hinging on the possibility of choosing a complete set of exact eigenstates in the form of scattering states, i.e., states of energy ϵ which describe a single particle "entering" the system in the transverse channel a of the ith lead and scattered with probability amplitude $t_{ia,jb}$ into any transverse channel b of the jth lead.

Within this mathematical assumption, the transmission coefficient T_{ij} that appears in Eq. (4) is found to be given by

$$T_{ij} = \sum_{a,b}|t_{ia,jb}|^2. \quad (21)$$

We refer to the original papers[14,15] for the details of this derivation. What is important for our purposes is that the conventional Landauer formula (4) emerges from an approximation to the exact formula (16)—an approximation in which only the first term in the infinite series of diagrams for the proper current-current response function is retained.

The question now arises how to go beyond this simplest approximation to include electron-electron interaction effects. In Sec. III we describe an approach based on time-dependent current-density-functional theory.

III. TIME-DEPENDENT CURRENT-DENSITY FUNCTIONAL THEORY

As discussed in Sec. I, a popular approach to the inclusion of many-body effects in nanoscopic transport is to use the Landauer formula (4), but calculate the transmission probabilities by solving the one-particle scattering problem in a static effective potential that includes many-body effects. How is such a potential to be constructed?

The ground-state DFT of Kohn and co-workers[36] offers a practical answer. According to this theory it is possible to find, in principle, an exchange-correlation potential which, in combination with the Hartree potential and the external potential, produces the correct ground-state density of the many-body system. Furthermore, this potential (known as the Kohn-Sham potential) is uniquely determined by the density. Thus, it is very tempting to make use of the Kohn-Sham potential to calculate the transmission probabilities and hope that all many-body effects pertaining to the transport problem be included. Unfortunately, this approach lacks any rigorous theoretical foundation. In practice, it amounts to "dressing up" the free particle lines in the first diagram of Fig. 2, while still discarding all the other diagrams. Therefore, it must be interpreted as nothing more than a single-particle *mean-field* approximation even if we knew the *exact* ground-state xc functional and as such there is no physical reason why this should be even approximately correct.

The time-dependent current-density-functional theory offers a more solid basis to attack the problem. Taking for granted the ordinary DFT description of the ground state, the TDCDFT attempts to describe the current response of the many-body system as the response of a noninteracting reference system to an effective time-dependent vector potential. The noninteracting reference system is usually taken to be the "Kohn-Sham system," i.e., the noninteracting system that is used in ordinary DFT to reproduce the ground-state density of the many-body system. Thus, in the TDCDFT approach the current response to a time-periodic vector potential $\mathbf{A}(\mathbf{r},t)=\mathbf{A}(\mathbf{r},\omega)e^{-i\omega t}+\text{c.c.}$ is written as

$$j_\alpha(\mathbf{r},\omega) = -e^2\sum_\beta\int d\mathbf{r}'\chi_{s,\alpha\beta}(\mathbf{r},\mathbf{r}';\omega) \times\{A_\beta(\mathbf{r}',\omega)+A_{H,\beta}(\mathbf{r}',\omega)+A_{\text{xc},\beta}(\mathbf{r}',\omega)\}, \quad (22)$$

where $\chi_{s,\alpha\beta}(\mathbf{r},\mathbf{r}';\omega)$ is the current response function of the Kohn-Sham system, $\mathbf{A}_H$ is the Hartree vector potential, and $\mathbf{A}_{\text{xc}}$ is the exchange-correlation vector potential.[37] The essential point is that the exchange-correlation potential is a unique functional of the current density and in the linear approximation can be represented as

$$-e^2A_{\text{xc},\alpha}(\mathbf{r},\omega) = \int d\mathbf{r}'\sum_\beta f_{\text{xc},\alpha\beta}(\mathbf{r},\mathbf{r}';\omega)j_\beta(\mathbf{r}',\omega), \quad (23)$$

where the "exchange-correlation kernel" $f_{\text{xc},\alpha\beta}(\mathbf{r},\mathbf{r}';\omega)$ is determined by the ground-state density. Later we will also need the "exchange-correlation electric field," which is defined as

$$E_{\text{xc},\alpha}(\mathbf{r},\omega) = i\omega A_{\text{xc},\alpha}(\mathbf{r},\omega). \quad (24)$$

The above formula (22) should be compared with the exact linear-response formula (17). Combining Eqs. (22), (23), and (17) we find the well-known relation between $\tilde{\chi}$, χ_s, and f_{xc}, namely,

$$[\tilde{\chi}^{-1}]_{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega) = [\chi_s]^{-1}_{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega) - f_{\text{xc},\alpha\beta}(\mathbf{r},\mathbf{r}',\omega), \quad (25)$$

where $[\tilde{\chi}^{-1}]_{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega)$ is the matrix inverse of $\tilde{\chi}_{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega)$, which is regarded as a matrix with indices $\alpha,\mathbf{r}$ and $\beta,\mathbf{r}'$.

Equation (25) gives us a handle on the inverse of the conductivity, i.e., the resistivity tensor. To make the connection, observe that the complex conductivity tensor $\tilde{\sigma}(\mathbf{r},\mathbf{r}',\omega)$ is given by

$$\tilde{\sigma}_{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega) = -e^2\frac{\tilde{\chi}_{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega)}{i\omega}, \quad (26)$$

whose real part reduces to $\sigma(\mathbf{r},\mathbf{r}')$ in the limit $\omega\to 0$. Accordingly, the complex resistivity tensor is given by

$$\tilde{\rho}_{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega) \equiv [\tilde{\sigma}^{-1}]_{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega) = -\frac{i\omega}{e^2}[\tilde{\chi}^{-1}]_{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega). \quad (27)$$

Then, making use of Eq. (25) we find

$$\tilde{\rho}_{\alpha\beta}(\mathbf{r},\mathbf{r}',\omega) = \tilde{\rho}_{s,\alpha\beta}(\mathbf{r},\mathbf{r}',\omega) + \frac{i\omega}{e^2}f_{\text{xc},\alpha\beta}(\mathbf{r},\mathbf{r}',\omega), \quad (28)$$

where the "Kohn-Sham resistivity," $\tilde{\rho}_s$, has the same relation to χ_s as the full interacting resistivity to $\tilde{\chi}$. Finally, taking the real part of both sides and going to the zero-frequency limit we find

$$\rho_{\alpha\beta}(\mathbf{r},\mathbf{r}') = \rho_{s,\alpha\beta}(\mathbf{r},\mathbf{r}') + \rho_{\mathrm{xc},\alpha\beta}(\mathbf{r},\mathbf{r}'), \tag{29}$$

where

$$\rho_{\mathrm{xc},\alpha\beta}(\mathbf{r},\mathbf{r}') \equiv - \lim_{\omega\to 0} \frac{\omega}{e^2} \Im m f_{\mathrm{xc},\alpha\beta}(\mathbf{r},\mathbf{r}',\omega). \tag{30}$$

This is the main result of our paper which we have anticipated in Eq. (6). We clearly see that the resistivity of the Kohn-Sham system—a noninteracting system in which many-body effects enter only implicitly through the static exchange-correlation potential—is not the whole story. This means, in particular, that it is not possible to give an exact representation of the conductance in terms of single-particle transmission probabilities. We have demonstrated this point for the linear-response regime, namely, in the limit of zero external bias. However, this result must be valid also out of linear response, even though in this case the extent of the dynamical corrections, which in linear response are embodied in $f_{\mathrm{xc},\alpha\beta}$, is not so easily determined.

We now shift our attention to the estimate of the dynamical exchange-correlation contribution ρ_{xc} which is controlled entirely and explicitly by many-body effects, i.e., time-dependent correlations in the effective potential of TDCDFT. The many-body kernel f_{xc}, which appears in Eq. (29), is not known exactly for any system, but a local approximation to it is available and has been used in the recent literature with varying degrees of success.[12,22,26,27,38] In a local approximation the key quantity

$$\tilde{E}_{\mathrm{xc},\alpha}(\mathbf{r},\omega) = -\frac{i\omega}{e^2}\sum_{\beta}\int d\mathbf{r}' f_{\mathrm{xc},\alpha\beta}(\mathbf{r},\mathbf{r}',\omega) j_{\beta}(\mathbf{r}',\omega), \tag{31}$$

which has the physical significance of "exchange-correlation electric field" [see Eq. (24)], is taken to be a function of the local value of $\mathbf{j}(\mathbf{r})$ and its first and second spatial derivatives. The simplest approximation in this class is the so-called adiabatic local-density approximation (ALDA), which provides an instantaneous connection between $\tilde{\mathbf{E}}_{\mathrm{xc}}(\mathbf{r})$ and $\mathbf{j}(\mathbf{r})$. In this approximation, however, f_{xc} is purely real, resulting in an exchange-correlation electric field that is always 90° out of phase with the current density. Therefore, such a field cannot contribute to the dc resistivity, consistent with the fact that $\Im m f_{\mathrm{xc}}$ vanishes in this approximation.

So in order to obtain exchange-correlation corrections to the resistivity we must go beyond the adiabatic approximation. This can be done with the help of the VK local-density approximation,[12] which calls into play the viscosity of the electron gas. In this approximation the exchange-correlation field has a dissipative component which is 180° out of phase, i.e., opposite to the current. In the zero-frequency limit this component of the exchange-correlation field has the form[13]

$$\begin{aligned} E_{\mathrm{xc},\alpha}(\mathbf{r}) &= -\sum_{\beta}\int d\mathbf{r}' \rho_{\mathrm{xc},\alpha\beta}(\mathbf{r},\mathbf{r}') j_{\beta}(\mathbf{r}') \\ &\simeq \frac{1}{e^2 n(\mathbf{r})}\sum_{\beta}\partial_{\beta}\left\{\eta(\mathbf{r})\left[\partial_{\beta}\left(\frac{j_{\alpha}(\mathbf{r})}{n(\mathbf{r})}\right) + \partial_{\alpha}\left(\frac{j_{\beta}(\mathbf{r})}{n(\mathbf{r})}\right)\right.\right. \\ &\quad \left.\left. - \frac{2}{3}\nabla_{\mathbf{r}}\cdot\left(\frac{\mathbf{j}(\mathbf{r})}{n(\mathbf{r})}\right)\delta_{\alpha\beta}\right]\right\}, \end{aligned} \tag{32}$$

where $\mathbf{j}(\mathbf{r})$ is the *electric* current density and $\eta(\mathbf{r})$ is the dc shear viscosity of a homogeneous electron gas of density $n(\mathbf{r})$.[25] Eqs. (29), (30), and (32) constitute a complete (albeit approximate) formulation of the microscopic resistivity tensor within TDCDFT. The Kohn-Sham resistivity itself is accessible from the ordinary static DFT. ρ_{xc} is best described through the effective electric field it produces—an electric field $\mathbf{E}_{\mathrm{xc}}$ directed *against* the current, which therefore does negative work on the current. In Sec. IV we show how our expression for $\mathbf{E}_{\mathrm{xc}}$ can be directly applied to the calculation of the macroscopic conductance.

IV. PERTURBATIVE CALCULATION OF THE CONDUCTANCE

Let us return to the system shown in Fig. 1 and assume that the electrochemical potentials μ_i are periodically modulated in time with a (very) small angular frequency ω. By "small" we mean a frequency much smaller than any other internal frequency of the system. The lead currents induced by the modulation are then also periodic and given by Eq. (1). Since the reservoirs are the only part of the system on which we have direct control it is evident that the work done on the system per unit time is

$$W = \sum_{i=1}^{N} \langle I_i \mu_i \rangle, \tag{33}$$

where the angular brackets denote a time average over a period of oscillation. This is also the energy that must be internally dissipated if the system is to remain in the steady state.

In order to express W in terms of the lead currents we must invert the linear relation (1) between the lead currents and the electrochemical potentials. Strictly speaking, this relation is not invertible because a rigid shift of all the electrochemical potentials has no effect on the current. But the problem is easily solved by permanently grounding one of the reservoirs, say, the one with $i=1$ so that $\mu_1=0$ at all times. Then the linear relation between the remaining $N-1$ currents $I_2,\ldots,I_N$ and the corresponding electrochemical potentials $\mu_2,\ldots,\mu_N$ *is* invertible, and the current in the grounded lead is simply given by $I_1=-I_2-\ldots-I_N$.

Then, we see that the dissipated power can be represented as

$$W = \sum_{i,j=2}^{N} \langle I_i R_{ij} I_j \rangle, \tag{34}$$

where the $(N-1)\times(N-1)$ matrix R_{ij} is the inverse of the matrix G_{ij} stripped of the first row and the first column.[39] The macroscopic expression for W in terms of R_{ij} is now equated to the usual microscopic expression in terms of the resistivity, resulting in the following equation:

$$\sum_{i,j=2}^{N} I_i R_{ij} I_j = \int d\mathbf{r}\int d\mathbf{r}' \mathbf{j}(\mathbf{r})\cdot\overleftrightarrow{\rho}(\mathbf{r},\mathbf{r}')\cdot\mathbf{j}(\mathbf{r}'), \tag{35}$$

where the integrals run over the volume of the system, including the leads, and we have dropped the time average by going to the zero-frequency limit. Finally, by making use of Eq. (29) we arrive at

$$\sum_{i,j=2}^{N} I_i R_{ij} I_j = \int d\mathbf{r} \int d\mathbf{r}' \mathbf{j}(\mathbf{r}) \cdot [\overleftrightarrow{\rho}_s(\mathbf{r},\mathbf{r}') + \overleftrightarrow{\rho}_{\mathrm{xc}}] \cdot \mathbf{j}(\mathbf{r}'). \tag{36}$$

This equation is formally exact if we know the exact many-body kernel f_{xc}. Let us compare it with the formula we would obtain from the conventional single-particle theory, i.e., from the Landauer formula (4), *for the same lead currents*.

As discussed in Sec. II, the "single-particle" theory assumes that all many-body effects can be included in the Kohn-Sham potential of the ground state. Apart from this, the system is noninteracting. The current-density distribution $\mathbf{j}_s(\mathbf{r})$ of this fictitious Kohn-Sham system is in general different from the true current-density distribution $\mathbf{j}(\mathbf{r})$ of the many-body system, even though the macroscopic lead currents, i.e., the fluxes of $\mathbf{j}$ and $\mathbf{j}_s$ into the leads, are imposed to be the same. Therefore, we write

$$\sum_{i,j=2}^{N} I_i R_{s,ij} I_j = \int d\mathbf{r} \int d\mathbf{r}' \mathbf{j}_s(\mathbf{r}) \cdot \overleftrightarrow{\rho}_s(\mathbf{r},\mathbf{r}') \cdot \mathbf{j}_s(\mathbf{r}'), \tag{37}$$

where $R_{s,ij}$ are the macroscopic resistances of the Kohn-Sham system obtained from the standard single-particle theory. Notice that the dynamical term $\overleftrightarrow{\rho}_{\mathrm{xc}}$ is absent in the single-particle theory.

The comparison between Eqs. (36) and (37) is complicated, in general, by the difference between $\mathbf{j}$ and $\mathbf{j}_s$. A simple comparison becomes possible in the perturbative limit, i.e., under the assumption that the dynamical many-body correction embodied in $\overleftrightarrow{\rho}_{\mathrm{xc}}$ is small. To this end we observe two facts: (i) The difference between $\mathbf{j}$ and $\mathbf{j}_s$ is of first order in the xc correction and (ii) the right-hand side of Eq. (37) is stationary under a small variation of the current distribution, such as the difference between $\mathbf{j}$ and $\mathbf{j}_s$. The physical reason for this is that in any linear system with external leads (such as the Kohn-Sham system we are considering here) the power dissipated is stationary with respect to an infinitesimal variation of the current distribution at *constant* lead currents. This implies that a first-order variation in the current distribution (about the steady distribution $\mathbf{j}_s$ in this case) produces a second-order variation in the dissipated power. Taking this into account we see that we can safely replace $\mathbf{j}_s$ by $\mathbf{j}$ in Eq. (37) and subtracting from Eq. (36) we arrive at the main result of this section:

$$\sum_{i,j=2}^{N} I_i \Delta R_{ij} I_j = \int d\mathbf{r} \int d\mathbf{r}' \mathbf{j}_s(\mathbf{r}) \cdot \overleftrightarrow{\rho}_{\mathrm{xc}}(\mathbf{r},\mathbf{r}') \cdot \mathbf{j}_s(\mathbf{r}'), \tag{38}$$

where

$$\Delta R_{ij} \equiv R_{ij} - R_{s,ij} \tag{39}$$

is the dynamical correction to the resistance. This equation expresses the many-body correction to the macroscopic resistance in terms of two things that are approximately known and/or calculable, namely, the resistivity exchange-correlation kernel $\overleftrightarrow{\rho}_{\mathrm{xc}}$, defined by Eq. (32), and the Kohn-Sham current distribution of the device, $\mathbf{j}_s(\mathbf{r})$, associated with the macroscopic lead currents I_i. The latter can be calculated, in principle, from the response of a noninteracting system to a screened electric field. In practice, one can calculate the correction to R_{ij} by considering a special situation in which only I_i and I_j are different from zero. Then the left-hand side of Eq. (38) gives us exactly the desired correction to R_{ij}.

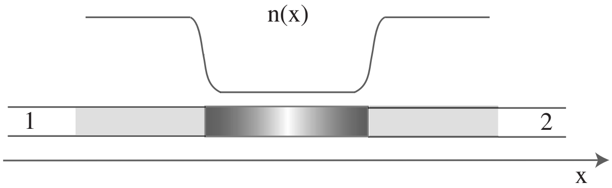

FIG. 3. A model two-terminal device in which the density changes only in one dimension. 1 and 2 are the lead regions.

V. EXAMPLE

Let us consider a simple model application of the general formalism. Our system is a potential barrier connected by two identical homogeneous leads (labeled 1 and 2 in Fig. 3) to two reservoirs, a "source" and a "drain," aligned along the x axis. The system is perfectly homogeneous in the transverse directions y and z. The density changes only in the x direction. The source (terminal 1) is grounded, so we only need to determine the two-terminal resistance R_{22} or, equivalently, the conductance $G_{22}=R_{22}^{-1}$. Let I be the current through the device and $\mathbf{j}(x)=I/A$ the current density, where A is the transverse cross section of the device.

Notice that in this case there is no question of $\mathbf{j}(x)$ being different from $\mathbf{j}_s(x)$ since, by continuity, they are both uniform and equal to I/A. In the absence of electron-electron interactions the conductance of this system is simply given by Eq. (4)—the total transmission probability across the potential barrier being the sum of the transmission probabilities of all the occupied transverse modes. Including the electron-electron interaction has two effects. The first is fairly trivial, namely, the effective potential in the ground state is modified by screening and exchange-correlation effects and the transmission probabilities must be recalculated for this effective potential. Up to this point the single-particle formula (4) remains in force.

The second effect is the dynamical exchange-correlation correction—an effect that cannot be forced into the mold of the static mean-field theory. Making use of Eq. (38) with $N=2$ and $j(x)=I/A$ we obtain

$$\Delta R_{22} = \frac{1}{A^2} \int d\mathbf{r} \int d\mathbf{r}' \rho_{\mathrm{xc}}(x,x'), \tag{40}$$

where $\rho_{\mathrm{xc}}(x,x')$ denotes the xx component of the tensor $\overleftrightarrow{\rho}_{\mathrm{xc}}(x,x')$ and we emphasize the fact that, due to our assumptions, it depends only on x and x'. Now observe that, according to Eq. (32) the action of ρ_{xc} on a uniform current density is specified by

$$\int d\mathbf{r}'\rho_{\mathrm{xc}}(x,x') = -\frac{4}{3e^2 n(x)}\partial_x\left[\eta(x)\partial_x\frac{1}{n(x)}\right], \qquad (41)$$

where $\eta(x)$ is the shear viscosity of the homogenous electron gas evaluated at the ground-state density $n(x)$. Substituting this in Eq. (40) and doing an integration by parts we arrive at

$$\Delta R_{22} = \frac{4}{3e^2 A}\int dx\,\eta(x)\frac{[n'(x)]^2}{[n(x)]^4}, \qquad (42)$$

where $n'(x)=\partial_x n(x)$. Notice that this has the correct dimensions of resistance because n is a three-dimensional density and η has the dimensions of $\hbar$ times a density. Figure 3 shows the electronic density in the leads and in the device. Clearly the dynamical correction comes entirely from the nonhomogeneous regions near the edges of the barrier (the contacts).

Equation (42) was first obtained in Ref. 22 in a more intuitive manner. The advantage of the present formulation is that it allows easy extension to more complicated situations. For example, we can include the dependence of the density on the transverse coordinates y and z, while neglecting variations of the transverse components of the current. In this case, we still have $\mathbf{j}(\mathbf{r})=\mathrm{const}$, but now the gradient of the density has both longitudinal and transverse components. As a result we get

$$\Delta R_{22} = \frac{1}{e^2 A^2}\int d\mathbf{r}\,\eta(\mathbf{r})\left\{\frac{4}{3}\frac{|\nabla_{\parallel} n(\mathbf{r})|^2}{[n(\mathbf{r})]^4} + \frac{|\vec{\nabla}_{\perp} n(\mathbf{r})|^2}{[n(\mathbf{r})]^4}\right\}, \qquad (43)$$

where $\nabla_{\parallel}$ is the x component of the gradient and $\vec{\nabla}_{\perp}$ is the gradient in the $y-z$ plane. This result (for constant viscosity) was first reported in Ref. 27 following an intuitive procedure, still based on the calculation of the power dissipated in the circuit.

VI. DISCUSSION AND CRITIQUE

In this paper we have shown that the single-particle mean-field framework of Landauer is inadequate *in principle* to describe the transport problem in nanoscale systems. That is to say a calculation of conductance from Eq. (4) would not provide the exact current even if one could determine the transmission probabilities with the utmost precision. Dynamical many-body effects enter the picture due to the *intrinsic* nonequilibrium nature of conduction.[1] These effects cannot be captured by a static formulation.

The next question is: what is the actual size of these dynamical corrections? One of the main results of this paper, Eq. (38), opens the way to a fully microscopic first-principles calculation of nanoscopic resistances and conductances (in the linear regime) within the framework of the local approximation to time-dependent current-density-functional theory. In Ref. 22 we tried to address this question for the simple quasi-one-dimensional model discussed in Sec. V and found that the viscosity correction to the resistance was only a small fraction of the total. For the case of two infinite jellium electrodes separated by a vacuum gap, a more accurate calculation based on the homogeneous electron-gas viscosity reported in Ref. 25 (see Fig. 4) showed an even smaller effect.[26] But, as pointed out in Sec. I, this does not mean that the issue is settled.

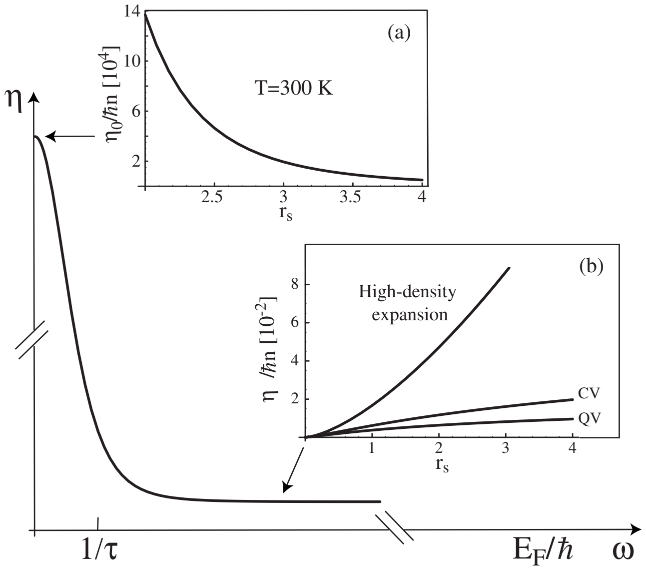

FIG. 4. Qualitative behavior of the viscosity of a homogeneous electron gas as a function of frequency. For frequencies smaller than $1/\tau$, with τ the quasiparticle relaxation time, η approaches the dc limit η_0. η_0 vs density is shown in inset (a) for $T=300$ K. The calculation is done with the Abrikosov-Khalatnikov formula (Ref. 40). For frequencies larger than $1/\tau$, but still much smaller than the Fermi frequency $E_F/\hbar$, η tends to a different constant η_∞. The behavior of η_∞ vs density is shown in inset (b) in various approximations at zero temperature. CV is from Ref. 25 and QV is from Ref. 41. The atomic unit of viscosity is $\hbar/a_B^3 = \simeq 7\times10^{-3}$ P (a_B is the Bohr radius) and $na_B^3 = 3/4\pi r_s^3$.

Looking back at Eq. (38) we see that an accurate evaluation of the viscosity correction has two ingredients: (1) the Kohn-Sham current-density distribution and (2) the viscosity of the homogeneous electron gas. As for the current density, it is important to note that all the estimates so far have been based on an oversimplified model in which the current density was assumed to be uniform in space.[22,26,27] In general, the spatial variation of the current density cannot be neglected especially in nanoscale systems where large transverse variations of the current density are common.[28–31]

Another and more fundamental source of uncertainty is in the value of the electronic viscosity which enters the dissipative kernel ρ_{xc}. The viscosity we have used so far, which is plotted in inset (b) of Fig. 4, was obtained from a zero-temperature calculation in the limit of zero frequency. In other words, the temperature (and, with it, the quasiparticle scattering rate) went to zero *before* the frequency. When calculated in this manner, the viscosity turns out to be very small indeed: its value is in the range of $10^{-5}/r_s^3$ P, where $r_s=(3/4\pi n a_B^3)^{1/3}\simeq 1$ is the average interelectron distance in units of the Bohr radius a_B. (For comparison, water at room temperature has a viscosity of about 10^{-2} P).

On the other hand, it is well known from the theory of homogeneous Fermi liquids[40] that the behavior of the viscosity is quite different if the zero-frequency limit is approached at finite temperature. Namely, in this case the viscosity turns out to be proportional to the mean-free path of the quasiparticles, which grows as $1/T^2$ in the low-temperature limit. The divergence of the zero-frequency viscosity for $T \to 0$ reflects the fact that long-lived quasiparticles can transport momentum arbitrarily far away from the source of the stress. This is also the reason why the viscosity of an ideal classical gas is independent of density,[42] since an increase or a decrease in the frequency of molecular collisions is exactly compensated by an opposite variation in the molecular mean-free path.

Panel (a) of Fig. 4 shows the behavior of the zero-frequency viscosity at room temperature for an electron gas in three dimension (3D), estimated from Eq. (7.22) of Ref. 40 with due allowance made for the different form of the interaction potential [the Abrikosov–Khalatnikov (AK) work was for ^{3}He]. Equation (7.22) of Ref. 40 can be rewritten as

$$\eta_0 = \hbar n \frac{8}{15\pi}\left(\frac{E_F}{k_B T}\right)^2 (k_F a_B)^2 \times \left\{\left[\frac{\bar{w}(\theta,\phi)}{\cos\frac{\theta}{2}}(1-\cos\theta)^2 \sin^2\phi\right]_{\text{av}}\right\}^{-1}, \tag{44}$$

which shows explicitly the physical dimensions of the viscosity ($\hbar n$). Here k_F is the Fermi wave vector, $E_F = \frac{\hbar^2 k_F^2}{2m}$ is the Fermi energy, a_B is the Bohr radius, and $\bar{w}(\theta,\phi)$ is the square of the matrix element of the electron-electron interaction potential (expressed in units of $4\pi e^2/k_F^2$) between the initial and final states of a collision process with incoming momenta $\mathbf{p}_1, \mathbf{p}_2$ and outgoing momenta $\mathbf{p}_1', \mathbf{p}_2'$, where θ is the angle between the incoming momenta and ϕ is the angle between the planes formed by $(\mathbf{p}_1, \mathbf{p}_2)$ and $(\mathbf{p}_1', \mathbf{p}_2')$. All the momenta are close to the Fermi surface and the symbol av denotes the average over θ and ϕ. The simplest approximation for $\bar{w}$ is the Thomas-Fermi approximation, in which we have

$$\bar{w}(\theta,\phi) = \left(\frac{1}{2(1-\cos\phi) + 4\alpha r_s/\pi}\right)^2, \tag{45}$$

with $\alpha = (4/9\pi)^{1/3} \simeq 0.521$. With this approximation, the average over θ can be done analytically and Eq. (44) can be rewritten as

$$\frac{\eta_0}{\hbar n} = \frac{1}{8(\alpha r_s)^6}\left(\frac{1.579 \times 10^5}{T}\right)^2 \times \left\{\int_0^\pi d\phi \frac{\sin^2\phi}{\left(4\sin^2\frac{\phi}{2} + \frac{4\alpha r_s}{\pi}\right)^2}\right\}^{-1}. \tag{46}$$

The result of the evaluation of this expression is shown in inset (a) of Fig. 4 for $T = 300$ K (room temperature). Notice that the presence of the factor $1/r_s^6$ causes the viscosity to increase sharply with increasing density, in contrast with what we observe in inset (b) of Fig. 4. It is evident that the dc viscosity is orders of magnitude larger than the finite frequency viscosity plotted in inset (b) of Fig. 4.

What does this imply for our analysis of the conductance in nanoscopic and mesoscopic devices? Obviously, these systems do not host a uniform electron liquid, and in particular they do not support long-lived quasiparticles that can transport momentum to infinity. This means that the large finite-temperature results of the uniform electron liquid are almost certainly not relevant for nanoscale devices: the mean-free path of quasiparticles is naturally limited by the geometric size of the device (see Appendix K of Ref. 1 and footnote 17 of Ref. 43). However, the huge difference between the numerical values of the viscosities in the insets of Fig. 4 suggests the possibility of a mesoscopic "middle ground" which under certain conditions may be much larger than the zero-temperature viscosity. This, however, is unlikely to be "universal," rather it must be related to the specific geometry of the system. A related difficulty is that, in general, the rate of dissipation in an interacting electron system depends strongly on the excitation spectrum of the system. Modeling dissipation through the viscosity of a homogeneous electron gas, as implied by our local-density approximation, may lead to a severely distorted description of the dissipative process. A truly universal description of dissipation (if possible at all) is still out of sight.

A central issue emerges from the above discussion, namely, the need for an accurate, testable, and reliable dissipative functional for time-dependent current-density-functional theory. The local-density approximation is only a first step. However, once a better functional is proposed, our formalism provides a simple and elegant way to test its predictions for the resistance of nanoscale systems.

Finally, we stress that we have focused our attention to the linear-response regime. It would be interesting and important (although not trivial) to extend the results presented in this paper to the nonlinear case. Obviously, a full-fledged *ab initio* calculation of transport using TDCDFT (as done, e.g., in Refs. 29 and 31) can always be performed. However, analytical results out of linear response are not available. Such an extension would allow analysis of the many-body corrections to the current-voltage characteristics—and corresponding dissipation—of nanoscale systems. It is particularly important for those instances, discussed above, in which the viscosity in nanostructures turns out to be much larger than that reported in Ref. 25.

ACKNOWLEDGMENTS

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