Conductance and polarization in quantum junctions

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We revisit the expression for the conductance of a general nanostructure—such as a quantum point contact—as obtained from the linear-response theory. We show that the conductance represents the strength of the Drude singularity in the conductivity $\sigma(k,k';i\omega\rightarrow0)$. Using the equation of continuity for electric charge we obtain a formula for conductance in terms of polarization of the system. This identification can be used for direct calculation of the conductance for systems of interest even at the *ab initio* level. In particular, we show that one can evaluate the conductance from calculations for a finite system without the need for special "transport" boundary conditions.

I. INTRODUCTION

The conductance gives the current as a linear response to an applied voltage for a given finite sample, specified by its atomic geometry. Typically, the sample of interest may be a thin chain of metallic atoms or a single molecule attached to metallic electrodes. The usual theory for *ab initio* prediction of conductances for these nanoscale devices is based on the Landauer formula[1]

$$G = \frac{2e^2}{h} T(e_F), \qquad (1)$$

which identifies the conductance with the transmission probability for an electron at the Fermi level $T(e_F)$ to penetrate the sample.

Given the impressive success of the Landauer-Büttiker equations[2] in many mesoscopic phenomena, many authors tried to relate it to basic principles. Since we are concerned with linear response, the general Kubo linear-response formalism[3] is well suited to this purpose. Among the first to do so were Economou and Soukoulis[4] who presented a derivation for noninteracting electrons. This was subsequently vigorously discussed,[5–7] since perfect transmission $T=1$ results in a finite conductance, not infinite as might be expected. Eventually the debate was reconciled with the realization that formula (1) gives the conductance between *reservoirs* and $2e^2/h$ represents an unavoidable minimum contact resistance if such macroscopic electrodes are connected through a quasi-one-dimensional (1D) contact. However, there are no such electrodes in the Kubo-like derivations, as has been pointed out by Landauer,[8] and so the result remained somewhat puzzling. The argument in favor of a Kubo-like derivation was an introduction of an auxiliary external field acting in the leads that compensates exactly the charge-density oscillations produced by the homogeneous field in the sample, resulting in the "four-point" conductance formula[5,6]

$$G^{4P} = \frac{2e^2}{h} \frac{T(e_F)}{1 - T(e_F)} \qquad (2)$$

that relates the current to the local drop in total electrostatic potential. However, in many experiments and situations it is

the two-point conductance G that is required, in which case formula (1) is frequently used for conductance calculations (e.g., for nanowires and metal-molecule-metal junctions). Therefore, clarification of the relationship of this formula to the Kubo approach remains necessary, and may lead to practical advances for *ab initio* calculations.

Much of the confusion arising from the "boundary and bulk contribution to the conductivity" introduced by the ideal leads has been clearly resolved by Sols[9] who emphasized the importance of global charge conservation and its relation to gauge transformations. In that paper, however, only the result (1) was derived and discussed and the induced charge-density oscillations were ignored.

The fundamental understanding of conductance as quantum-mechanical transmission relies on the picture of distinct electrochemical potentials for the two electrodes. These dictate the occupation of states in the nonequilibrium sample. An alternative point of view (equally valid but much closer to the Kubo formalism) is that of electrons accelerated in the applied external field. The ability of the field to accelerate electrons in extended or bulk materials has been used by Kohn[10] to distinguish between conductors and insulators where conductors are characterized by $\lim_{\omega\rightarrow0} \mathrm{Im}\{\sigma(\omega,q=0)\}\sim A/\omega, A\neq0$, and the case $A=0$ characterizes insulators. This point of view, but applied to conductance of finite samples or mesoscopic conductors, has been considered by Fenton[11] who strictly differentiated between a localized external field leading—through acceleration of electrons over a finite distance—to a finite conductance and yielding the Landauer formula, and a homogeneous field giving a response characteristic of the bulk material with ω^{-1} singularity. An approach based on coupled self-consistent equations for the current density, electron density, and induced field, implicitly also representing the "conductance based on acceleration" point of view, was set out in detail by Kamenev and Kohn.[12] They focus on the four-point conductance, which they define as the current divided by *induced* potential drop, thereby completely neglecting the electrostatic drop in the external potential. This is appropriate in some cases, since a finite constant external field over infinitely long leads contributes negligibly to the total potential drop around the sample. It is

important to note that their self-consistent field is obtained from the 1D Poisson equation, i.e., a system resembling parallel planes of charge e moving along their normal rather then electrons confined to a 1D wire. The former systems has far stronger screening behavior then the latter. More detailed calculations by Sablikov and Shchamkhalova,[13] who also used the Kubo formalism, show that the effective interaction between electrons in an 1D wire is not strong enough to screen the charge and a uniform current coexists with an induced dipole moment of the electron density in the wire.

In this paper we derive a formula for the steady-state conductance in terms of the irreducible polarization of the system of interest. Our starting point is application of an external field and following the time evolution for large times. We will show that only the $q=0$ Fourier component of the field influences the steady-state current because the nonlocal conductivity is a sharply peaked function of q, eventually becoming a Dirac δ function. *The weight of this δ function has directly the meaning of conductance.* At the same time, this singular behavior also corresponds to the Drude singularity $\mathrm{Im}\{\sigma(\omega)\} \sim \omega^{-1}$ if we set $q=0$ and then take the limit $\omega \to 0$. It is interesting to note that from this point of view we can identify the conductance with the Drude weight, a connection encountered in somewhat different circumstances in the conductive properties of extended systems.[14] In addition to providing an interpretation of the conductance, our formula is suitable for practical *ab initio* calculations. Using the continuity equation we circumvent the need for matrix elements of current operator, which are in general difficult to evaluate numerically, and express the conductance in terms of the irreducible polarization at small imaginary frequency—a quantity that can be evaluated efficiently even using *ab initio* methods that describe electronic correlation.[15,16]

II. CONDUCTANCE IN IMAGINARY FREQUENCY

Consider a system, infinitely long along the x direction and finite, infinite or periodic along the other two perpendicular directions. Along the x axis we apply an infinitesimally weak external electric field. The response of the system will be in general nonlocal in time and space, and quantitatively described by the Kubo linear-response theory:[3]

$$\mathbf{j}(\mathbf{r},t) = \int_{-\infty}^{t} \vec{\vec{\sigma}}(\mathbf{r},\mathbf{r}';t-t') \cdot \mathbf{E}(\mathbf{r}',t')d^3r'dt', \quad (3)$$

$$\vec{\vec{\sigma}}(\mathbf{r},\mathbf{r}';t) = i\Theta(t)\int_{0}^{-i\beta} d\tau \mathrm{Tr}\{\rho_{eq}\mathbf{j}(\mathbf{r}',t+\tau)\mathbf{j}(\mathbf{r},0)\}, \quad (4)$$

where $\mathbf{j}(\mathbf{r},t)$ is the current density, $\mathbf{E}(\mathbf{r},t)$ external electric field, $\vec{\vec{\sigma}}(\mathbf{r},\mathbf{r}';t)$ nonlocal tensor of conductivity, $\Theta(t)=1$ for $t>0$ and $\Theta(t)=0$ otherwise, and ρ_{eq} the equilibrium density matrix.

We take the form of the field as $E_x(\mathbf{r},t)=E(x)\Theta(t), E_y = E_z = 0$. Introducing the current $I(x,t)=\int d\mathbf{S} \cdot \mathbf{j}(\mathbf{r},t)$ (where we integrate over the surface perpendicular to x) and utilizing our particular choice of external field we obtain

$$I(x,t) = \int dx' I_\sigma(x,x';t)E_x(x'), \quad (5)$$

$$I_\sigma(x,x';t) = \int_{-\infty}^{t} dt' \int d\mathbf{S} \cdot \vec{\vec{\sigma}}(\mathbf{r},\mathbf{r}';t') \cdot d\mathbf{S}'. \quad (6)$$

In the steady state we are interested in the limit $t \to \infty$ so that for the steady-state current we have

$$I_\sigma(x,x') = \lim_{\alpha \to 0^+} \int_{-\infty}^{\infty} dt' e^{-\alpha t'} \sigma(x,x';t') = \sigma(x,x';\omega=i0^+), \quad (7)$$

where we have introduced the effective one-dimensional conductivity $\sigma(x,x';\omega)=\int d\mathbf{S} \cdot \vec{\vec{\sigma}}(\mathbf{r},\mathbf{r}';\omega) \cdot d\mathbf{S}'$. The positive infinitesimal α plays an important role for systems without dissipation, where application of a field for an infinitely long time results in the system being heated. This is avoided by introducing an effective finite (but large) measurement time $T \sim \alpha^{-1}$. In this way we avoid the heating problem because we first let $E(x) \to 0$ (linear response) and only afterwards $\alpha \to 0^+$. [Identical expressions are obtained assuming adiabatic switching on of the external field $E(x,t)=E(x)e^{\alpha t}$ as t approaches 0 from below, and measuring the current at $t=0^-$, which is the more conventional point of view.]

We are principally concerned with the total current I and not the current density. Similarly, we would like to work with the bias voltage $V=\int d\mathbf{r} \cdot \mathbf{E}(\mathbf{r})=\int dxE(x)$ rather than the field itself. To achieve this we Fourier transform with respect to x

$$I(q) = \int \frac{dq'}{2\pi} \sigma(q,q')E(q'), \quad (8)$$

$$\sigma(q,q') = \int e^{-iqx+iq'x'} \sigma(x,x')dxdx'. \quad (9)$$

First, the steady-state current needs to be independent of x, $I(x)=I$, as a consequence of the equation of continuity, so that $I(q)=2\pi I\delta(q)$ and therefore directly also $\sigma(q,q') \sim \delta(q)$. Second, as a direct consequence[9] of the linearity of the theory, the steady-state current is uniquely given by the bias $V=E(q=0)$ only. This means that for two external fields $E(q)$ and $E'(q)$ whose long-range parts are equal $[E(q=0)=E'(q=0)]$, but otherwise are arbitrary, one has to obtain identical steady-state currents. We therefore conclude that $\sigma(q,q') \sim \delta(q')$ in the limit $\alpha \to 0^+$, i.e., it is a sharply peaked function of q' so that, based on Eq. (8), it is only the values of $E(q)$ or $E'(q)$ at $q=0$ that affect the steady current. Using these observations in Eq. (8) we obtain

$$G = \frac{I}{V} = \int \frac{dqdq'}{4\pi^2} \sigma(q,q'), \quad (10)$$

or using the fact that $\sigma(q,q') \sim \delta(q)\delta(q')$ we can also write

$$\lim_{\alpha \to 0^+} \sigma(q,q';i\alpha) = 4\pi^2 G\delta(q)\delta(q'). \quad (11)$$

This is one of the central results of this paper and directly shows that conductance is the strength or weight of the

Drude singularity. Formula (10) can be used for extrapolative evaluation of the conductance from the conductivity at small imaginary frequencies, and since it is peaked function in q, q', the conductivity needs to be evaluated for small values of these variables only. We will demonstrate this approach numerically in Sec. V.

III. CONDUCTIVITY AND POLARIZATION

Evaluation of the conductance using Eq. (10) requires calculation of the Fourier transform of the conductivity. The latter is, in a real-space representation, given by Eq. (4) which itself is difficult to evaluate for all necessary $\mathbf{r}, \mathbf{r}'$. On the other hand, substantial experience has been accumulated in calculations of the polarization $\chi(\mathbf{r}, \mathbf{r}'; t)$, defined by[15,16]

$$\chi(\mathbf{r}, \mathbf{r}'; t - t') = \frac{\delta n(\mathbf{r}, t)}{\delta V(\mathbf{r}', t')}, \qquad (12)$$

where $\delta n(\mathbf{r}, t)$ is a change in density due to infinitesimally weak external potential $V(\mathbf{r}, t)$. To relate these two we utilize the equation of continuity integrated over the cross-sectional area

$$\partial_x I(x, t) = \partial_t N(x, t). \qquad (13)$$

From the definition of the polarization we have $N(x, t) = \int_0^t dt' \int dx' \chi(x, x'; t - t') V(x, t')$, where our $\chi(x, x'; t)$ is now, similarly to $\sigma(x, x'; t)$, integrated across the cross-sectional area [$d\mathbf{S}$ and $d\mathbf{S}'$ integrals in Eq. (6)]. Substituting the linear-response formulas for current (5) and density $N(x, t)$, Fourier transforming into q, q' variables and using the fact that the external potential is arbitrary, we immediately obtain

$$\sigma(q, q'; i\alpha \to i0^+) = \lim_{\alpha \to 0^+} \frac{\alpha}{qq'} \chi(q, q'; i\alpha). \qquad (14)$$

We note that the singular character of $\sigma(q, q')$ for small q, q' as given in Eq. (11) does not arise fundamentally from the $1/qq'$ prefactor, since $\chi(q, q'; \omega) \approx qq' f(q, q'; \omega)$ where $f(0, 0) \neq 0$. This property is a consequence of conservation of total number of particles [$n(q=0) = N$] or the absence of response in density if we change the potential everywhere by a constant $q' = 0$.

Expressing the conductance through the polarization is particularly suited to a correct treatment of a system of interacting electrons. In the first place, it is crucial to define the conductance not as a coefficient for current dependence on the external but on the total electric field $\mathbf{E}^t(\mathbf{r}) = \mathbf{E}(\mathbf{r}) + \mathbf{E}^i(\mathbf{r})$. The induced field $\mathbf{E}^i(\mathbf{r})$ can be obtained from Poisson equation

$$i(q\hat{\mathbf{x}} + \mathbf{G}) \cdot \mathbf{E}^i(q, \mathbf{G}; t) = -4\pi \delta n(q, \mathbf{G}; t), \qquad (15)$$

where $\hat{\mathbf{x}}$ is a unit vector in the x direction and $\mathbf{G}$ is a 2D reciprocal lattice vector corresponding to the perpendicular coordinates. Using the linear-response result for $\delta n(q, \mathbf{G}; t)$ in terms of $\chi(\mathbf{r}, t)$ [see Eq. (12)] we arrive at the relation between the total and external field

$$\mathbf{E}^t(q, \mathbf{G}) = \int dq' \left[\hat{\mathbf{x}} \delta_{\mathbf{G}, 0} \delta(q - q') \right.$$
$$\left. + \frac{q\hat{\mathbf{x}} + \mathbf{G}}{q'} \frac{4\pi}{q^2 + |\mathbf{G}|^2} \chi(q, \mathbf{G}; q', 0) \right] E(q'). \qquad (16)$$

If we multiply the latter equation by the unit vector $\hat{\mathbf{x}}$ and subsequently invert it for $\mathbf{G} = 0$, we obtain the relation between the external field $E(q)$ and the total field along $\hat{\mathbf{x}}$ averaged over the cross-sectional area $E^t(q, \mathbf{G} = 0)$. Substituting this relation into Eq. (8) we obtain, after some algebra (see first section of the Appendix),

$$G = \lim_{\alpha \to 0^+} \frac{\alpha}{4\pi^2} \int \frac{\chi^t(q, q'; i\alpha)}{qq'} dq dq', \qquad (17)$$

where we introduce the "*transport part of the polarization*," $\chi^t(q, q'; i\alpha)$, related to the irreducible polarization $\chi^0(q, \mathbf{G}; q', \mathbf{G}')$ through an equation of Dyson type

$$\chi^t(q, \mathbf{G}; q', \mathbf{G}') = \chi^0(q, \mathbf{G}; q', \mathbf{G}') + \int dk \sum_{\mathbf{K} \neq 0} \chi^t(q, \mathbf{G}; k, \mathbf{K})$$
$$\times \frac{4\pi}{k^2 + |\mathbf{K}|^2} \chi^0(k, \mathbf{K}; q', \mathbf{G}'). \qquad (18)$$

The corrections entering through $\mathbf{K} \neq 0$ terms in Eq. (18) are known as local-field effects in the context of evaluation of the macroscopic dielectric function.[16] Here, however, it is not quite the same since $k = 0, \mathbf{K} \neq 0$ part is included into χ^t whereas for the macroscopic dielectric function the sum is restricted to $k \neq 0, \mathbf{K} \neq 0$. The omission of the $\mathbf{K} = 0$ term involving $4\pi/k^2$ in Eq. (18) stems directly from the fact that it is precisely this term that converts the drop in external field into drop in the total field, as can be seen from Eq. (16) when taking into account that the drop in total field is given by $\Delta V^t = E^t(q = 0, \mathbf{G} = 0)$. Correct evaluation of the conductance in 3D therefore requires inclusion of these "perpendicular" local-field effects, included within χ^t but not in χ^0, into account. Essentially, χ^t describes the response of the density to the effective potential, except that long-range screening of the potential in the x direction is specifically excluded, allowing the conductance to address the applied voltage rather than the local potential drop.

For systems translationally invariant along the perpendicular directions, $\chi^0(q, \mathbf{0}; k, \mathbf{G}) \sim \delta_{\mathbf{0}, \mathbf{G}}$ and the last term in Eq. (18) becomes identically zero. It follows that in this particular case $\chi^t = \chi^0$ and the conductance of noninteracting electrons, defined with respect to drop in the *external* field, is identical to the conductance of interacting electrons, treated within the random-phase approximation (RPA), defined with respect to drop in the *total* field.

IV. LANDAUER FORMULA

In this section we present simple, analytically tractable cases that illustrate the theory of the preceding sections. Consider first the case of noninteracting electrons in a quantum wire with only one subband. It is well known that the polarization function has the form[17]

$$\chi(q,q';\omega) = \frac{1}{2\pi q} \ln \left[\frac{\omega^2 - (q^2/2 - k_F q)^2}{\omega^2 - (q^2/2 + k_F q)^2} \right] \times 2\pi\delta(q - q'),$$

$$(19)$$

where the factor $2\pi\delta(q-q')$ arises trivially from the translational invariance of the system along the x axis. Using this expression in Eq. (14) immediately gives $\sigma(q,q';i\alpha \to i0^+) = 2\pi\delta(q')\delta(q)$ and therefore through Eq. (11) $G = 1/2\pi$, the quantum of conductance (i.e., e^2/h in SI units). Using Eq. (17) without application of the limit, and Eq. (19), it is also possible to obtain the analytical dependence of conductance G on imaginary frequency $\alpha = -i\omega$ for this system,

$$G(\alpha) = \frac{1}{\sqrt{2}\pi(1 + \sqrt{1 + [\alpha/e_F]^2})^{1/2}}. \quad (20)$$

This functional form will be extremely useful for numerical calculation of $G(0^+)$ based on extrapolation to zero frequency, described in Sec. V.

It is also instructive to explore the behavior of $I_\sigma(t \to \infty)$ directly [see Eq. (6)]. The latter can be calculated, e.g., using Fourier transform of Eq. (19)

$$\begin{aligned} I_\sigma(q,q';t) &= \int_0^t dt' \, \sigma(q,q';t') \\ &= \int_0^t dt' \frac{\partial_{t'}\chi(q,q';t')}{qq'} \\ &= \frac{\chi(q,t)}{q^2} \times 2\pi\delta(q - q'), \end{aligned} \quad (21)$$

where we have used the expression (14) in the real-time domain. The result is

$$I_\sigma(q,q';t) = \frac{2}{\pi q^3 t} \sin(k_f q t)\sin\left(\frac{q^2}{2}t\right)\Theta(t) \times 2\pi\delta(q - q'),$$

$$(22)$$

which for $t \to \infty$ evidently approaches the form (11) with $G = 1/2\pi$. The lesson from these analytical examples is that the well-known formulas for polarization can be used for evaluation of the conductance of the system, and that the limit $i\omega \to 0^+$ clearly corresponds to the steady-state limit $t \to \infty$.

Because the conductivity is sharply peaked around $q' = 0$, only the $q = 0$ component of the applied field E has an effect on the total current. This allows us to include, as a limiting case, a homogeneous field. For a system with a constant field applied over length L, the field itself must be $\sim 1/L$ so that we have a sufficiently small finite drop $V = \int_L E dx \sim 1$. The physical meaning of the finite conductance of a scattering-free segment of a metallic wire is clearly a manifestation of the free acceleration of electrons over the distance L. This is in agreement with the point of view advocated by Fenton.[11] However, there is no need to keep L strictly finite; in fact the limiting case $L \to \infty$ can be still characterized by a finite overall conductance by taking careful limits and using properties of the Dirac δ function, as mentioned above for the case of the free-electron gas [following Eq. (22)]. In simple terms, this represents the limit of increasing the length over which
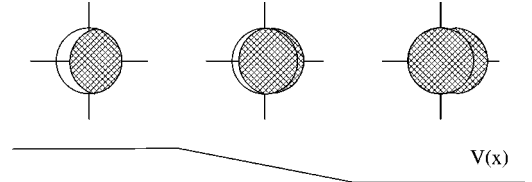

FIG. 1. Semiclassical interpretation of a finite-field potential $V(x)$ applied to a wire. The local Fermi spheres are depicted as for 2D gas for clarity. The filled area on top of the equilibrium spheres indicates accelerated electrons, while the empty area inside the equilibrium spheres represents states emptied by the decelerating effect of the uphill field.

the external field is applied, L, while decreasing the intensity of the field E in such a way as to keep the drop $V \sim EL$ finite and small.

A simple qualitative demonstration of this argument can be made semiclassically. Consider a finite drop over finite region of a 1D wire as shown in Fig. 1. The current can be obtained from the local Fermi distribution on the far right. Electrons that are occupying states above the equilibrium distribution have travelled to the right from the region with an accelerating field. These, during their flight through the region, gained energy ΔV so that they represent current $I = 1/L\Sigma_k k_F$ where we sum over states with accelerated electrons, i.e., $k: e_k \in (e_F, e_F + \Delta V)$. This obviously leads to the quantum of conductance $G = 1/2\pi$. While formally we have striking similarity with the usual "two chemical potentials" picture, it should be noted that the microscopic interpretation of these expressions is different. As can be seen from Fig. 1, the local charge neutrality is clearly violated in the constant potential regions on the right and left while in the center it is locally charge neutral where the distribution corresponds to the shifted Fermi sphere. The infinite L limit, discussed in previous paragraph, resolves this problem by sending the regions with unbalanced local charge away into infinities.

When we insert a localized scattering potential characterized by the transmission matrix

$$\mathbf{T}(k) = \begin{bmatrix} r(k) & \tilde{r}(k) \\ t(k) & \tilde{r}(k) \end{bmatrix} \quad (23)$$

into 1D gas of electrons, the Landauer formula is obtained. We obtain the desired demonstration of the sharply peaked character of $\sigma(q,q';i\alpha)$ by analytically continuing Kamenev and Kohn's expression[12] onto the imaginary frequency axis,

$$\sigma(q,q';i\alpha) = \frac{1}{2\pi} \left\{ \frac{2k_F\alpha}{k_F^2 q^2 + \alpha^2} 2\pi\delta(q - q') \right.$$

$$\left. - |r(e_F)|^2 \frac{2k_F\alpha}{k_F^2 q^2 + \alpha^2} \frac{2k_F\alpha}{k_F^2 q'^2 + \alpha^2} \right\} \quad (24)$$

$$\to 2\pi|t(e_F)|^2 \delta(q)\delta(q'). \quad (25)$$

Alternatively, we can arrive at the same result using Eq. (17), which explicitly shows the utility of reformulation of transport through the polarization function in imaginary frequency. A detailed derivation is given in the second section of the Appendix.

We stress that this result for the *two*-point conductance (1) of noninteracting electrons also applies to interacting electrons if the conductance is defined with respect to the total field at the RPA level of approximation. The four-point conductance (2) may be formulated in a similar fashion, which, if combined with the approximate effective electron-electron interaction $v_{ee}^{1D}(q) \sim 1/q^2$, would be equivalent to the treatment of Kamenev and Kohn.[12] (In their calculation the four-point conductance is defined as $G^{4P} = I/V^i$, where V^i is the self-consistent induced drop only. The reason for neglecting the drop in external field is due to the above mentioned limiting procedure; since $E \times L$ is finite while $L \to \infty$, $E \times L'$ will be negligible for any finite L'. Since the four-point measurement is meant across a finite distance L', the contribution to the total drop on finite distance comes solely from the induced field.)

V. FEASIBILITY FOR NUMERICAL CALCULATIONS

The expression for the conductance (17), together with some experience gained from the evaluation of G for lead-scattering-lead system in the Appendix, motivates the following suggestion: can the correct conductance of an infinite system be calculated using a finite system with some arbitrary boundary conditions, determining the polarization as a function of α, and then extrapolating $\alpha \to 0$?

For the purpose of this exploration we have considered a square-barrier potential in 1D, for which the results for transmission coefficients are well-known analytically. We calculate the polarization function using the Green's function of the equilibrium system given by equation

$$[e - \hat{H}(x)]\mathcal{G}(x,x';e) = \delta(x-x'), \tag{26}$$

supplemented by the chosen boundary conditions. For simplicity and for the purpose of illustration, we take the extreme case of "zero-boundary" conditions on the wave functions.[18] In this case, it is clear that $G(\alpha) \to 0$ as $\alpha \to 0$. In terms of the Green's function we can easily express the polarization as

$$\chi(x,x';i\alpha) = \sum_{i}^{occ} [\mathcal{G}(x,x';e_i + i\alpha)\phi_i(x')\phi_i^*(x)$$
$$+ \mathcal{G}(x',x;e_i - i\alpha)\phi_i(x)\phi_i^*(x')], \tag{27}$$

where we sum over occupied states only, and ϕ_i are eigenstates of $\hat{H}$ from Eq. (26). The Green's function at given energy is found by direct integration of Eq. (26) and eigenstates are easily found by matching plane waves with the chosen boundary conditions. Finally we use a discrete Fourier transform, $\chi(x,x') \to \chi(K,K')$, to obtain the estimate of conductance

$$G(\alpha) = \sum_{K,K'} \alpha \frac{\chi(K,K';i\alpha)}{KK'}. \tag{28}$$

The discrete Fourier transform introduces a convergence parameter: the real-space step size Δx or, equivalently, number of discretization points N. Altogether, the calculation
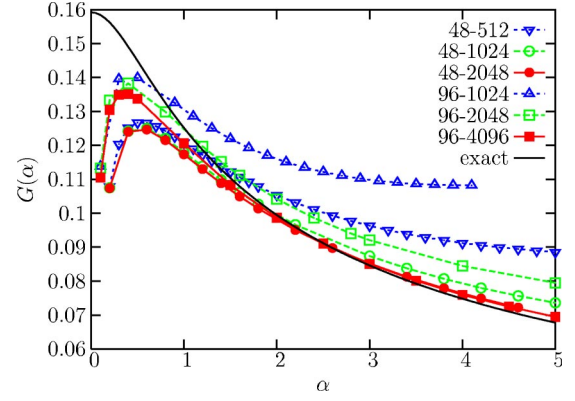

FIG. 2. The dependence of conductance of free-electron 1D gas on imaginary frequency. Black line corresponds to the analytical result (20) and the numerical data labels "*L-N*" represent system of length L a.u. with N discretization points in real space. Apart from the low-energy drop to zero, which is characteristic of a finite system, the functions converge to the exact result for the infinite system. This opens the possibility of calculating the dc conductance by extrapolation from moderate values of α.

needs to be converged with respect to the system size L and with respect to N, and extrapolated with respect to imaginary energy α.

Before we discuss results for nonzero barrier height, let us first consider the case of zero barrier height, i.e., the free-electron gas. In this case we know exactly the whole dependence of $G(\alpha)$, given by Eq. (20). We have fixed the Fermi wave vector to $k_F = \pi/3$ a.u., corresponding to $e_F \approx 0.5$ a.u. In Fig. 2 we show numerical results obtained using Eq. (28). The labels "*L-N*" represent system of length L a.u. with N discretization points in real space, or equivalently, the number of K points in the discrete Fourier transform. We obtain our chosen Fermi energy for lengths $L=48$ and 96 when occupying 16 and 32 states, respectively.

From Fig. 2 we see that the numerical results converge to the analytical expression for energies $\alpha \gg e_F$. The lower limit of this range can be brought closer to e_F by increasing the length of the system. However, for a longer system the convergence with respect to N becomes more demanding, with the error growing with energy. This behavior can be traced to the cusp in the polarization $\chi(x,x')$ at $x=x'$. It can be easily found from Eq. (27) that the size of this cusp is

$$\chi'(x,x')_{x=x'^+} - \chi'(x,x')_{x=x'^-} = 4\sum_{i}^{occ} \phi_i^*(x)\phi_i(x). \tag{29}$$

This expression could be used to remove the cusp from numerical Fourier transforms and substantially decrease the needed number of K points. In the present paper, since our system is computationally undemanding, we have instead simply increased N until satisfactory convergence was achieved.

Next we include a square barrier into our system. In Fig. 3 we show results of calculation with barrier with width $a=2$ a.u. and height e_F. In this case the transmission probability is approximately 50% which is indicated in the upper
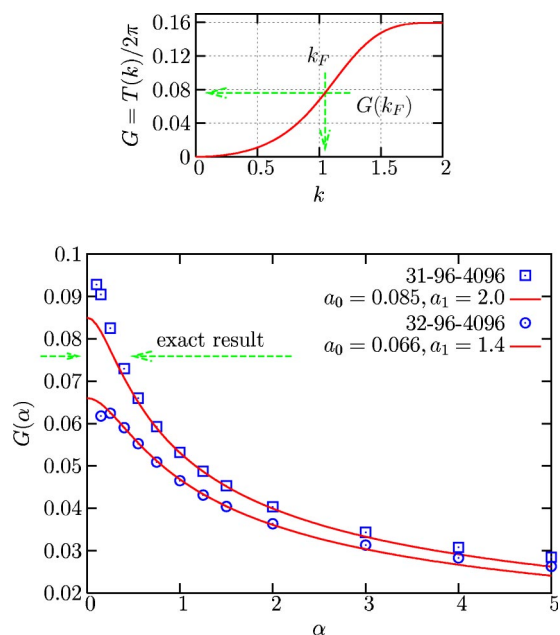
FIG. 3. The dependence of conductance, given by Landauer formula, on the Fermi energy ($k_F = \pi/3$ in our calculations) for a square barrier of height e_F and width $\lambda_F/3$ (upper graph) and the dependence of the numerically calculated conductance on the imaginary energy (lower graph). $G(\alpha)$ approaches the exact result of infinite system before it turns rapidly towards zero.

graph with arrows. In the lower graph we show the dependence of conductivity on the imaginary frequency α. The two sets of numerical data correspond to odd and even numbers of occupied states, converged with respect to N within the considered range of α. The convergence of data with respect to L is first fast but eventually becomes rather slow. In fact, it is not our aim to get the conductance of an "almost infinite" system, but rather to be able to extract the conductance of an infinite system from a calculation for a sufficiently large but finite system. The shown length $L=96$ a.u. is to be compared with the Fermi wavelength $\lambda_F \approx 6$.

A striking difference between odd and even number of occupied states comes from the fact that placing the barrier of length $a=2$ in the center affects the symmetric and antisymmetric states (at the Fermi energy) differently. Clearly, the former have a much larger amplitude at the scattering potential than the latter (which are zero in the center of the system) and therefore the symmetric states will be more affected. This is in agreement with the conductance for 32 occupied states being below that for 31 occupied states. For $L \to \infty$ these two states become degenerate and the difference between odd and even cease to exist. By bracketing the exact conductance in this way, we can obtain acceptable convergence even with the crude "zero" boundary conditions.

When calculating conductance we need to be able to extrapolate our data to zero energy. As we have pointed out above, the small-energy turnaround of G arises from the finite size of the system and we should not take that into account. To fit the data we have used a scaled version of the functional form obtained for the free gas,

$$G(\alpha) = \frac{a_0}{\sqrt{2}\pi(1 + \sqrt{1 + [2a_1\alpha]^2})^{1/2}}, \quad (30)$$

where a_0 and a_1 are fitting parameters, representing linear scaling of the conductance and energy axes. As we see from Fig. 3 the fit is very good over the crucial middle range of frequencies. For $\alpha > 3$ it becomes worse but we already know that this difference can be attributed to convergence problems with number of K points due to the cusp in $\chi(x, x')$. When looking at $\alpha \to 0$ limit of our fitted expressions (coefficients a_0 in Fig. 3) we see the values bracket the exact value with an relative error of roughly 10%. Averaging the result for even and odd states gives a smaller and more convergent error (0.5%).

This calculation is intended to be illustrative, yet it shows that the formula (17) can, in principle, lead to the correct answer even when applied to system with zero-boundary conditions. We particularly believe that the use of periodic boundary conditions will significantly improve the performance of this approach for the main problem of the zero-boundary condition is clearly the one-way transfer of charge from one side to the other, which introduces finite-system errors after a relatively short time, and therefore spoils $G(\alpha)$ between $\alpha=0$ and a relatively large value. This gross effect is not present for a periodic system.

VI. CONCLUSIONS

We have developed a unifying point of view of the polarization, the nonlocal conductivity and the conductance which supplies a steady-state transport characteristics of any system. We have shown that the weight of the Drude singularity at zero frequency of the nonlocal conductivity, when considered in reciprocal space, directly corresponds to the conductance of the system to which we apply a field with a nonzero overall drop in potential. We have identified a simple relation between conductivity and polarization for the case of a system under unidirectional external field that eventually led us to a simple formula for conductance, expressed through the polarization of the system at small imaginary frequency. Expressed in terms of polarization, it turned out to be possible to address the self-consistent field that contributes to the drop in total potential used for definition of conductance. We have shown that the formula for its evaluation remains formally intact but instead of the polarization function we need to supply a "transport part" of the polarization. The latter is identical to the irreducible polarization in 1D, but differs from it in general 2D or 3D systems except where perfect translational invariance exists perpendicular to the flow of current.

Finally we have demonstrated that our expression for conductance in terms of polarization can be used for the convenient numerical evaluation of the conductance for systems without imposing specific boundary conditions in the form of scattering states. This formulation is directly suitable for inclusion of many-body or inelastic effects, since it is based on the polarization function for which approximations that include these complications are very well developed.

Note added in proof. We are thankful to M. Büttiker for drawing our attention to his early account on the role of polarization in the treatment of conductance and total field in a model quantum junction.[19]

APPENDIX

1. Derivation of Eq. (17)

Let $g(q,q')$ be the inverse operator to the right-hand side in Eq. (16) for $\mathbf{G}=0$.

$$\int dk\, g(q,k)\left(\delta(k-q') - \frac{4\pi}{kq'}\chi(k,q')\right) = \delta(q-q'),$$

$$\text{(A1)}$$

so that $E(q) = \int dk\, g(q,k)E^t(k)$. According to Eq. (5) we have

$$I(q) = \int dk \int \frac{dq'}{2\pi} \frac{\alpha\chi(q,q')}{qq'} g(q',k)E^t(k), \quad \text{(A2)}$$

which motivates us to define

$$\chi^t(q,q') = q' \int dk \frac{\chi(q,k)}{k} g(k,q'). \quad \text{(A3)}$$

Multiplying Eq. (A1) with $q'\chi(q'',q)/q$ from left and integrating over q we have

$$\chi^t(q'',q') - 4\pi \int dk \frac{\chi^t(q'',k)}{k^2}\chi(k,q') = \chi(q'',q'), \quad \text{(A4)}$$

comparing term by term this Dyson-like equation with the Dyson equation for the reducible polarization $\chi(q,q')$ we arrive at Eq. (18) which omits the $\mathbf{K}=0$ term from the sum. Substitution of Eq. (A3) into Eq. (A2) give immediately the result (17) which concludes the stated results in Sec. III.

2. Derivation of Eq. (25) using formula (17)

The polarization of noninteracting electrons is given by expression[15]

$$\chi(q,q';i\alpha) = \sum_{ij} \langle i|e^{-iqx}|j\rangle\langle j|e^{iq'x}|i\rangle \frac{n_i - n_j}{i\alpha - e_j + e_i}, \quad \text{(A5)}$$

where $|i\rangle$ are eigenstates of the electronic Hamiltonian with eigenenergy e_i, n_i is its occupation factor and

$$\langle i|e^{-iqx}|j\rangle = \int dx\langle i|x\rangle e^{-iqx}\langle x|j\rangle. \quad \text{(A6)}$$

Using formula (10) we therefore have

$$G = \int \frac{dq\, dq'}{2\pi\, 2\pi} \sum_{ij} \langle i|\frac{e^{-iqx}}{q}|j\rangle\langle j|\frac{e^{iq'x}}{q'}|i\rangle \frac{\alpha(n_i - n_j)}{i\alpha - e_j + e_i}. \quad \text{(A7)}$$

The first two matrix elements are, after integrations, complex conjugate to each other and therefore their product is real.

The last fraction in Eq. (A7) is not state but energy dependent and its real part, which is only needed, is given by

$$\frac{\alpha}{(e_i - e_j)^2 + \alpha^2} \frac{dn(e_i)}{de_i}(e_i - e_j)^2. \quad \text{(A8)}$$

We have already used the fact that in the limit of our interest $(\alpha \to 0)$ the first factor will be sharply peaked and therefore we can use linear Taylor expansion of $n(e_j)$ around e_i. However, the expression will be nonzero only if the factor $(e_i - e_j)^2$ will be compensated by the energy dependence of the matrix elements, which we will confirm in following paragraphs.

In the next step we interchange the order of integrations in Eq. (A7) so that we directly evaluate

$$\int \frac{dq}{2\pi} \frac{e^{iqx}}{q + i\epsilon} = -i\Theta(-x)e^{\epsilon x}, \quad \text{(A9)}$$

where we interpret the singularity to be at $q = -i\epsilon$. This is in fact arbitrary since, as we have pointed out in Sec. III, $\chi(q,q';\omega) = qq'f(q,q')$. An equally valid choice of singularity at $q = +i\epsilon$ leads to identical results.

We can now finally turn to evaluation of the matrix elements. The asymptotic character of the wave functions has the well-known form

$$\phi_{k,R}(x) = \frac{1}{\sqrt{2\pi}} \begin{cases} e^{ikx} + r_k e^{-ikx} & x \ll 0 \\ t_k e^{ikx} & x \gg 0. \end{cases} \quad \text{(A10)}$$

$$\phi_{k,L}(x) = \frac{1}{\sqrt{2\pi}} \begin{cases} \tilde{t}_k e^{-ikx} & x \ll 0 \\ e^{-ikx} + \tilde{r}_k e^{ikx} & x \gg 0. \end{cases} \quad \text{(A11)}$$

The final integrals we need to do have the form

$$(k,R/L|k',R/L) = \int_{-\infty}^{0} e^{\epsilon x}\phi^*_{k,R/L}(x)\phi_{k',R/L}(x)dx, \quad \text{(A12)}$$

and of there we need to keep only those that are singular $\sim 1/k - k'$ since in Eq. (A8) we need to compensate the factor $(e_k - e_{k'})^2 = \frac{1}{2}(k+k')^2(k-k')^2$. Foreseeing the δ function character with respect to $e_k - e_{k'}$ and $e_k - e_F$ appearing in Eq. (A8) we can directly use $t_k = t_{k'} = t_{k_F}$ and $r_k = r_{k'} = r_{k_F}$, the transmission and reflection probability amplitudes at the Fermi energy, respectively. It is now easy to see that the singular terms are

$$(k,R|k',R) = -(k,L|k',L) = \frac{1}{2\pi}\frac{|t|^2}{k-k'}, \quad \text{(A13)}$$

$$(k,R|k',L) = (k,L|k',R)^* = \frac{1}{2\pi}\frac{r^*\tilde{t}}{k'-k}. \quad \text{(A14)}$$

Using these forms, together with Eq. (A8) and the form zero-temperature limit that $dn(e)/de = \delta(e - e_F)$ we directly get

$$G = \frac{1}{2\pi}(|t|^4 + |t|^2|r|^2) = \frac{|t|^2}{2\pi}, \quad \text{(A15)}$$

the celebrated Landauer formula.

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