Deconstructing Kubo formula usage: Exact conductance of a mesoscopic system from weak to strong disorder limit

Branislav K. Nikolić

Department of Physics, Georgetown University, Washington, DC 20057-0995
(Received 20 March 2001; published 1 October 2001)

In both research and textbook literature one often finds two "different" Kubo formulas for the zero-temperature conductance of a noninteracting Fermi system. They contain a trace of the product of velocity operators and single-particle (retarded and advanced) Green operators: $\mathrm{Tr}(\hat{v}_x \hat{G}^r \hat{v}_x \hat{G}^a)$ or $\mathrm{Tr}(\hat{v}_x \mathrm{Im}\, \hat{G} \hat{v}_x \mathrm{Im}\, \hat{G})$. The study investigates the relationship between these expressions, as well as the requirements of current conservation, through exact evaluation of such quantum-mechanical traces for a nanoscale (containing 1000 atoms) mesoscopic disordered conductor. The traces are computed in the semiclassical regime (where disorder is weak) and, more importantly, in the nonperturbative transport regime (including the region around localization-delocalization transition) where the concept of a mean free path ceases to exist. Since quantum interference effects for such strong disorder are not amenable to diagrammatic or nonlinear σ-model techniques, the evolution of different Green function terms with disorder strength provides insight into the development of an Anderson localized phase.

At first sight, the title of this paper might sound perplexing. What else can be said about Kubo formula[1] after almost a half of a (last) century of explorations in practice, as well as through numerous rederivations in both the research[2] and textbook[3,4] literature? Kubo linear response theory (KLRT) represents the first full quantum-mechanical transport formalism. It connects irreversible processes in nonequilibrium to the thermal fluctuations in equilibrium [fluctuation-dissipation theorem (FDT)]. Therefore, the study of transport is limited to the nonequilibrium states close to equilibrium. Nevertheless, the computation of linear kinetic coefficients is greatly facilitated since final expressions deal with equilibrium expectation values of relevant physical quantities (which are much simpler than the corresponding nonequilibrium ones[5]). It originated[6] from the Einstein relation for the diffusion constant and mobility of a particle performing a random walk.

Until the scaling theory of localization[7] and ensuing computation of the lowest-order quantum correction, weak localization[8] (WL), to the Drude conductivity, it almost appeared that the microscopic and complicated Kubo formulation of quantum transport merely served to justify the intuitive Bloch-Boltzmann semiclassical approach[3] to transport in weakly disordered ($k_F l \gg 1$, where k_F is the Fermi wave vector and l is the mean free path) conductors. Furthermore, the advent of mesoscopic physics[9] has led to a reexamination of major transport ideas—in particular, we learned how to apply properly KLRT to finite-size systems. Thus, equivalence was established[2] between the rigorous Kubo formalism and heuristically founded Landauer-Büttiker[10] scattering approach to linear response transport of noninteracting quasiparticles.[11] This has emerged as an important tool for studying mesoscopic transport phenomena, where system size and interfaces through which electrons can enter or leave the conductor play an essential role in determining the conductance.[12,13]

This study presents an exact evaluation of two different Kubo-type expressions for the linear conductance of a meso-scopic disordered conductor. Both expressions are frequently encountered in the research as well as textbook literature, and are displayed below. They consist of a trace (or linear combination of such traces) over the product of velocity operators $\hat{v}_x$ with retarded and advanced single-particle Green operators $\hat{G}^{r,a} = [E - \hat{H} \pm i0^+]^{-1}$, like $\mathrm{Tr}[\hat{v}_x \hat{G}^{r,a} \hat{v}_x \hat{G}^{r,a}]$, where $\hat{H}$ is an equilibrium Hamiltonian (in the spirit of FDT, it contains random and confining potentials, but not the external electric field), and the velocity operator is defined by $i\hbar \hat{\mathbf{v}} = [\hat{\mathbf{r}}, \hat{H}]$. These quantum-mechanical traces are computed here, Figs. 1 and 2, in the site representation (i.e., using real-space Green functions) defined by a lattice model, such as the tight-binding Hamiltonian (TBH)

$$\hat{H} = \sum_{\mathbf{m}} \varepsilon_{\mathbf{m}} |\mathbf{m}\rangle \langle \mathbf{m}| + \sum_{\langle \mathbf{m}, \mathbf{n} \rangle} t_{\mathbf{mn}} |\mathbf{m}\rangle \langle \mathbf{n}| \tag{1}$$

on a hypercubic lattice N^d of size $L = Na$ (a being the lattice constant). Here $t_{\mathbf{mn}}$ is the nearest-neighbor hopping integral between s orbitals $\langle \mathbf{r} | \mathbf{m} \rangle = \psi(\mathbf{r} - \mathbf{m})$ on adjacent atoms located at sites $\mathbf{m}$ of the lattice ($t_{\mathbf{mn}} = 1$ inside the sample defines the unit of energy). The disorder is simulated by taking a random on-site potential such that $\varepsilon_{\mathbf{m}}$ is uniformly distributed over the interval $[-W/2, W/2]$, which is the so-called Anderson model of localization. I emphasize the requirements of current conservation throughout this analysis, which will allow us to understand the features of different trace expressions introduced above.

The mesoscopic methods (mesoscopic Kubo[2,14] or, equivalently, Landauer[10] formula) make it possible to get the exact zero-temperature (i.e., quantum) conductance of a finite-size sample attached to semi-infinite disorder-free leads. Although KLRT is a standard formalism for introducing the many-body physics into the computation of transport coefficients,[4] here the focus is on the transport properties determined by scattering of noninteracting (quasi)electrons on impurities. The "old" Kubo formula[15] for the macro-
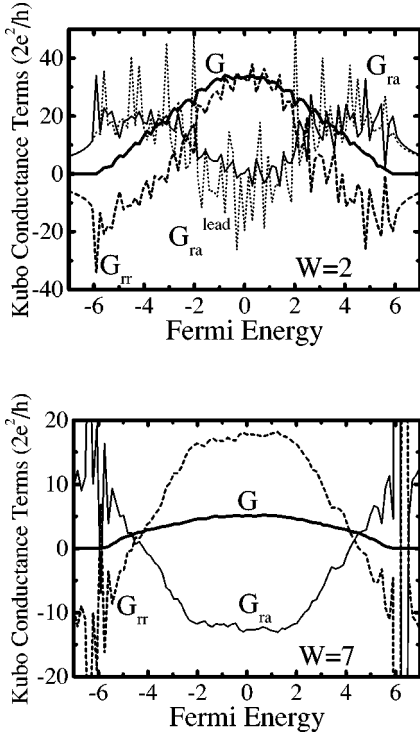
FIG. 1. Different terms in the Kubo formula for the two-probe quantum conductance of a single finite-size sample modeled on a simple cubic lattice 10^3 by an Anderson model with disorder strength $W=2$ (upper panel—single sample in the semiclassical transport regime) or $W=7$ (lower panel—disorder averaged over 50 samples in the nonperturbative transport regime $k_F l \lesssim 1$). The full Kubo conductance (thick solid line) is given by the sum of terms defined in Eq. (6) (thin solid line) and Eq. (7) (dashed line), $G = G_{ra} + G_{rr}$. The respective traces in these expressions are performed only over the states residing on the first two planes inside the sample. The dotted line in the upper panel represents G_{ra}^{lead} obtained by tracing over the two planes deep inside the left lead (at a distance $10a$ away from the sample).

scopic volume-averaged longitudinal dc conductivity at zero temperature ($E \equiv E_F$ in all formulas below, E_F being the Fermi energy) of a noninteracting Fermi gas described by a single-particle Hamiltonian $\hat{H}$ is given by

$$\sigma_{xx} = \frac{2\pi e^2 \hbar}{\Omega} \text{Tr}[\hat{v}_x \delta(E-\hat{H}) \hat{v}_x \delta(E-\hat{H})], \qquad (2)$$

where the factor of 2 accounts for the spin degeneracy. The Kubo conductivity relates the spatially averaged current $\mathbf{j} = \int d\mathbf{r} \, \mathbf{j}(\mathbf{r})/\Omega$ to the spatially averaged electric field $\mathbf{j} = \sigma \mathbf{E}$, where thermodynamic limit $\Omega = L^d \rightarrow \infty$ (while keeping the impurity concentration finite) is implied to get an unambiguous intensive quantity[16,7] (and well-defined steady state). For electrons in a random potential further averaging should be performed over the disorder to get σ as a material constant.[17] On the other hand, quantum corrections to the conductivity are nonlocal[8] on the scale of the dephasing length $L_\phi \gg l$. This invalidates the concept of local quantities, like conductivity, in mesoscopic samples, which are smaller than L_ϕ and thereby effectively at $T=0$. Therefore, mesoscopic transport
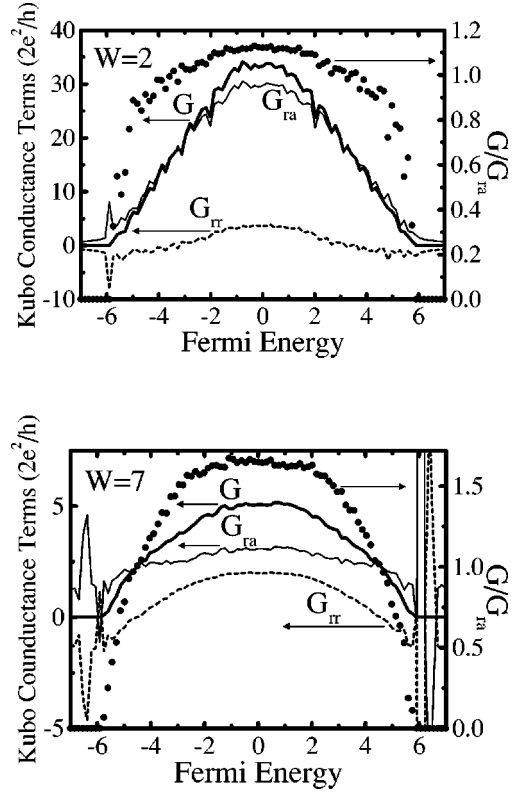

FIG. 2. Different terms in the Kubo formula $G = G_{ra} + G_{rr}$ for the two-probe quantum conductance of the same finite-size conductors as in Fig. 1, but with respective traces in these expressions performed over the site states inside the whole disordered sample.

has to be described in terms of sample-specific quantities, like conductance, which describe a given sample measured in a given manner[2] (i.e., more generally, conductance coefficients $I_p = \Sigma_q g_{pq} V_q$ in Ohm's law for a multiprobe geometry, where several leads are attached to the sample to feed the current I_p or measure the voltages V_q) or, alternatively, the nonlocal conductivity tensor introduced below. Switching to conductance leads to the following Kubo expression:

$$G = \frac{4e^2}{h} \frac{1}{L^2} \text{Tr}[\hbar \hat{v}_x \text{Im} \, \hat{G} \hbar \hat{v}_x \text{Im} \, \hat{G}], \qquad (3a)$$

$$\text{Im} \, \hat{G} = \frac{1}{2i}(\hat{G}^r - \hat{G}^a) = -\pi \delta(E-\hat{H}). \qquad (3b)$$

Here the definition of the retarded (r) or advanced (a) single-particle Green operator $\hat{G}^{r,a} = [E-\hat{H} \pm i0^+]^{-1}$ requires a numerical trick to handle the small imaginary part $i0^+$, which then spoils the prospect of obtaining the exact zero-temperature conductance.[18,19] Once the semi-infinite clean leads are attached to the finite sample (at planes 1 and N along x axis for a two-probe geometry, Fig. 3), the "self-energy" $\hat{\Sigma}^{r,a} = \hat{\Sigma}_L^{r,a} + \hat{\Sigma}_R^{r,a}$, arising from the "interaction" with the leads (L left, R right), provides a well-defined imaginary part in the definition of the Green operators[20]

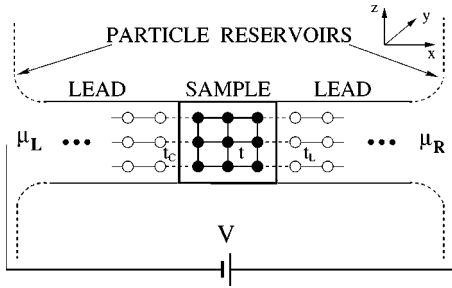$$\hat{G}^{r,a} = [E-\hat{H} - \hat{\Sigma}^{r,a}]^{-1}. \qquad (4)$$

FIG. 3. A two-dimensional (2D) version of the actual 3D model of the two-probe measuring geometry employed here. Each site hosts a single s orbital which hops to six (or fewer for surface atoms) nearest neighbors. The hopping matrix element is t (within the sample), t_L (within the leads), and t_C (coupling of the sample to the leads). The leads are semi-infinite and are considered to be connected at $\pm\infty$ to "reservoirs" biased by the potential difference $eV = \mu_L - \mu_R$.

The Green function $\hat{G}^{r,a}(\mathbf{n},\mathbf{m}) = \langle \mathbf{n}|\hat{G}^{r,a}|\mathbf{m}\rangle$ describes the propagation of electrons between two sites inside an open conductor ($L_\phi = L$ in the two-probe geometry). The self-energy terms are given[20,21] by $\hat{\Sigma}_{L,R}^r(\mathbf{n},\mathbf{m})$ $=(t_C^2/2t_L^2)\hat{g}_{L,R}^r(\mathbf{n}_S,\mathbf{m}_S)$ with $\hat{g}_{L,R}^r(\mathbf{n}_S,\mathbf{m}_S)$ being the surface Green function of the bare semi-infinite lead between the sites $\mathbf{n}_S$ and $\mathbf{m}_S$ located on the end atomic layer of the lead (and adjacent to the corresponding sites $\mathbf{n}$ and $\mathbf{m}$ inside the conductor). It has an imaginary part only for $|E| \leq 6t_L$, which means that $G(E_F)$ goes to zero at the band edge of a clean lead $|E_F| = 6t_L$ because there are no states in the leads beyond this energy which can carry the current. Here the leads will be described by the TBH with $\varepsilon_\mathbf{m} = 0$ and $t_\mathbf{mn} = t_L$; the hopping between the sites in the lead and the sample is $t_\mathbf{mn} = t_C$, as illustrated in Fig. 3.

I use the term "mesoscopic Kubo formula" for Eq. (3) with the Green operators (4) plugged in. This formula is exactly equivalent[2] to a two-probe Landauer formula[10] for the conductance measured between two points deep inside macroscopic reservoirs to which the leads are attached at infinity.[22] Thus, it is conceptually different from the "plain" Kubo formula (2) which follows from combining the conductance of smaller parts $G = \sigma L^{d-1}/L$, thereby implying a local description of transport which becomes applicable only at sufficiently high temperatures. Such mesoscopic formulas provide a means to compute the quantum conductance—a sample-specific quantity which takes into account the finite system size, measuring geometry, arrangement of impurities, and nonlocal features of quantum transport and can describe ballistic transport (where the local relation $\mathbf{j} = \sigma\mathbf{E}$ does not hold). Attempts to use the original Kubo formulas on finite samples, throughout the premesoscopic history[18,19] of the Anderson localization theory, were thwarted with ambiguities, which can be traced back to the general questions on the origin of dissipation.[23] This stems from the fact that a stationary regime cannot be reached unless the system is infinite or coupled to a thermostat. From the practical point of view, leads make the system infinite by opening the sample and therefore eliminating the technical obstacles in handling of the discrete spectrum of finite samples.[24] Furthermore, the

use of semi-infinite leads allows us to bypass explicit modeling of reservoirs in the computation of conductance since "hot" electrons which escape into the leads (due to the broadening of energy levels) do not come back in a phase-coherent fashion. The concept of reservoirs was always an essential part of Landauer's subtle arguments.[23] They provide dissipation and therefore the steady state.[27] However, the computation of conductance, as a measure the dissipation, involves only a conservative Hamiltonian of noninteracting electrons scattered on impurities (i.e., when computing the linear conductance of a mesoscopic system one usually does not deal explicitly with electron-electron and electron-phonon interactions[11]).

The conductance computed from the mesoscopic quantum expression is exact, but characterizes the whole *sample +leads* system in the spirit of quantum measurement theory since leads can also be considered as the "macroscopic measuring apparatus."[25,26] However, for a disordered enough sample (and not too narrow leads or too small t_C) the conductance is determined mostly by the disordered region itself.[28,21] This exactness makes it possible to compute the transport properties in both the semiclassical regime (where Boltzmann theory and perturbative quantum corrections are applicable since $k_F l \gg 1$) and the nonperturbative transport regime[29] where semiclassical concepts, like l, lose their meaning. Although the distinction between $k_F l \sim 1$ (where semiclassical theory, including the perturbative quantum corrections, breaks down) and the criterion $G \sim 2e^2/h$ for the localization-delocalization (LD) critical point has been known since the scaling theory of localization,[7] it is not uncommon practice to find these two different boundaries of transport regimes confused. As the disorder is increased, a sample goes from the semiclassical transport regime, through a vast region between $k_F l \sim 1$ and the LD transition (e.g., $6 \lesssim W \lesssim 16.5$ at $E_F = 0$ in the Anderson model[29]), and finally enters into a localized phase. Since the nonperturbative transport regime lacks the small parameter required by present analytical schemes, the numerical techniques employed here are the only way to gain insight into the quantum effects beyond the lowest-order corrections, like WL, or a resummation of all such perturbative quantum correction within the nonlinear σ-model formalism.[30,31]

Another expression is often encountered in the literature[3,16,5,20,32] for both the conductance of finite-size systems and conductivity of infinite systems. It gives the conductance through an apparently different trace, $G \propto \mathrm{Tr}[\hbar\hat{v}_x \hat{G}^r \hbar\hat{v}_x \hat{G}^a]$. While some textbooks quote this only as a convenient approximation to the disorder-averaged full formula,[3,16,5] sometimes the claim goes further to say that such a trace is equivalent to the Landauer formula, and moreover it can be evaluated at any cross section inside the disordered region, thus relaxing the requirement of perfect leads "as the weakest point of the Landauer formalism."[32] Namely, $\hat{G}^r\hat{G}^r$ or $\hat{G}^a\hat{G}^a$ terms can be reduced to a single Green function via the Ward identity in weakly disordered conductors,[33,3] and are therefore related to the density of states. They are "abandoned" in the limit $k_F l \gg 1$ since they do not generate interesting contributions to WL or meso-

scopic fluctuations [for example, such terms generate contribution to universal conductance fluctuations which are small as $\sim 1/(k_F l)^2$].[16] In fact, both the diffusion modes of the Diffuson-Cooperon diagrammatic perturbation theory and different versions of the nonlinear σ model (NLSM) are derived[25,31] by considering only the term containing the product $\hat{G}^r \hat{G}^a$. The NLSM is a quantum field theory[25] of weakly disordered mesoscopic conductors where diffusion modes of the diagrammatic perturbation theory play the role of soft modes responsible for long-range spatial correlations of local density of states, mesoscopic fluctuations of global quantities, and nonlocal corrections to conductivity.[34] It makes it possible to handle the breakdown of perturbation theory due to the proliferation of such modes[34] by summarizing all WL-type corrections to conductivity.[30] This then justifies the phenomenological one-parameter scaling theory[7] (if not rigorously, then at least qualitatively) and explains the LD transition in $2 + \epsilon$ dimensions where Anderson localization occurs at weak disorder $k_F l \gg 1$.

To remove possible confusion,[25] it should be emphasized that the conductance coefficients g_{pq}, obtained by integrating the Kubo nonlocal conductivity tensor $\underline{\sigma}(\mathbf{r}, \mathbf{r}')$ over the cross sections in the leads p, q,

$$g_{pq} = -\int_{S_p} \int_{S_q} d\mathbf{S}_p \cdot \underline{\sigma}(\mathbf{r}, \mathbf{r}') \cdot d\mathbf{S}_q, \tag{5}$$

also contain Im $\hat{G}$ for $p = q$, while for $p \neq q$ only the terms involving $\hat{G}^r \hat{G}^a$ are nonzero.[2] The cross sections S_p and S_q are to be chosen far enough from the sample, where all evanescent modes have died out. This not only provides a rigorous foundation for the Landauer formalism, but also clarifies some subtle points in the Kubo formalism (like disorder averaging[35] and independence of linear transport properties from the nonequilibrium charge redistribution[36]). By writing the full Kubo formula (3) as a sum $G = G_{ra} + G_{rr}$, I introduce the "Kubo conductance terms"

$$G_{ra} = \frac{2e^2}{h} \frac{1}{L^2} \text{Tr}[\hbar \hat{v}_x \hat{G}^r \hbar \hat{v}_x \hat{G}^a], \tag{6}$$

$$G_{rr} = -\frac{2e^2}{h} \frac{1}{L^2} \text{Tr}[\hbar \hat{v}_x \hat{G}^r \hbar \hat{v}_x \hat{G}^r]. \tag{7}$$

Obviously, if in some transport regime conductance can be obtained from the trace in G_{ra}, the other term G_{rr} has to vanish, at least approximately.

Before embarking on the direct evaluation of these expressions for a conductor described by TBH (1), the crucial point is to understand the way (i.e., space of states $|\mathbf{m}\rangle$) in which the traces should be performed, $\text{Tr}(\cdots) = \Sigma_{\mathbf{m}} \langle \mathbf{m}|(\cdots)|\mathbf{m}\rangle$. Naively, in the site representation it would appear that trace in formula (3) should include site states inside the whole sample. However, once the current conservation $\nabla \cdot \mathbf{j}(\mathbf{r}) = 0$ is invoked, this becomes extraneous. All Kubo conductivity or conductance formulas stem

from the more fundamental quantity in KLRT, the nonlocal conductivity tensor relating local current density to the local electric field,

$$\mathbf{j}(\mathbf{r}) = \int d\mathbf{r}' \, \underline{\sigma}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{E}(\mathbf{r}'). \tag{8}$$

This tensor is obtained as a response to an external field only since corrections to the current due to the field of induced charges go beyond the linear transport regime[37,38] (i.e., one does not have to engage in the much more cumbersome task of finding the response to a full electric field inside the conductor[4]). In application of KLRT to mesoscopic systems, $\underline{\sigma}(\mathbf{r}, \mathbf{r}')$ is a sample-specific quantity, i.e., defined for each impurity configuration and arrangement of the leads,[2] and is in fact nonlocal even after disorder averaging.[36] Because it is not directly measurable, some volume averaging is needed to get the quantities that can be related to experiments:

$$G = \frac{1}{V^2} \int_\Omega d\mathbf{r} \, d\mathbf{r}' \mathbf{E}(\mathbf{r}) \cdot \underline{\sigma}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{E}(\mathbf{r}'). \tag{9}$$

Here V is the bias voltage ($V \to 0$ in the linear transport regime), e.g., in the case of two-probe geometry $eV = \mu_L - \mu_R$, where leads are in equilibrium with two macroscopic reservoirs characterized by constant chemical potentials μ_L and μ_R (Fig. 3). Although this expression contains the local electric field $\mathbf{E}(\mathbf{r}) = \nabla \mu(\mathbf{r})/e$ inside the conductor, because of current conservation entailing $\nabla \cdot \underline{\sigma}(\mathbf{r}, \mathbf{r}') = \underline{\sigma}(\mathbf{r}, \mathbf{r}') \cdot \nabla' = 0$ (which is a special case, in the absence of magnetic field, of a more general theorem[2]), the conductance will not depend on these field factors.[35,36] In the case of TBH (1) with nearest-neighbor hopping the expectation value of the velocity operator in the site representation $\langle \mathbf{m}|\hat{v}_x|\mathbf{n}\rangle = (i/\hbar)t_{\mathbf{mn}}(m_x - n_x)$ is nonzero only between the states residing on adjacent planes [technical details of the route from Eq. (9) to the trace involving the velocity operator are meticulously covered in Ref. 2]. Thus, the minimal space choice here is defined by taking $\mathbf{E}(\mathbf{r})$ to be nonzero on two adjacent planes, while the standard textbook assumption of a homogeneous field[3,15] $|\mathbf{E}| = V/L$ throughout the sample leads to Eqs. (2) and (3). Blind tracing over the whole sample would give simply the conductance multiplied by the square of the number of pairs of adjacent planes, meaning that such a trace should be divided by $(N-1)^2 a^2$ to get G [when the trace is performed only over the arbitrary two adjacent planes, L^2 in Eq. (3) is replaced by a^2]. The physical content of this statement is simple: current $I = GV$ is the same on each cross section. Therefore, the conductance depends only on the total voltage drop over the sample, and not on the local current density and electric field distributions.

At this point, it is worth mentioning that another expression is frequently employed in the real-space computational practice. It stems from the linear response limit of a formula derived by the Keldysh technique (for noninteracting[39] or interacting systems[40]):

$$G = \frac{4e^2}{\pi\hbar} \mathrm{Tr}(\mathrm{Im}\,\hat{\Sigma}_L \hat{G}^r_{1N} \mathrm{Im}\,\hat{\Sigma}_R \hat{G}^a_{N1}). \qquad (10)$$

Here $\hat{G}^r_{1N}$, $\hat{G}^a_{N1}$ are the submatrices of the full Green function $\hat{G}^{r,a}(\mathbf{m},\mathbf{n})$ whose elements connect layer 1 to layer N of the sample. Therefore, only an $N^2 \times N^2$ block of the whole $N^3 \times N^3$ matrix $\hat{G}^r(\mathbf{n},\mathbf{m})$ is needed to compute the conductance. Although such "partial" knowledge of the whole Green function and the trace over matrices of size N^2 in Eq. (10) are different from the corresponding counterparts required in application of the mesoscopic Kubo formula (where the minimal trace goes over $2N^2 \times 2N^2$ matrices), the final result for the conductance is the same. Positive definiteness of the operators $-2\,\mathrm{Im}\,\hat{\Sigma}_{L,R}$ makes it possible to find their square root and recast the expression under the trace of Eq. (10) as a Hermitian operator. The expression (10) then looks like the two-probe Landauer formula involving a transmission matrix $\mathbf{t}$,

$$G = \frac{e^2}{\pi\hbar} \mathrm{Tr}(\mathbf{t}\mathbf{t}^\dagger) = \frac{e^2}{\pi\hbar} \sum_{n=1}^{N^2} T_n, \qquad (11)$$

$$\mathbf{t} = 2\sqrt{-\mathrm{Im}\,\hat{\Sigma}_L}\,\hat{G}^r_{1N}\sqrt{-\mathrm{Im}\,\hat{\Sigma}_R}, \qquad (12)$$

or transmission eigenvalues T_n when the trace is evaluated in a basis which diagonalizes $\mathbf{t}\mathbf{t}^\dagger$. Moreover, it is more efficient from a practical point of view since the Green function techniques used to evaluate Eq. (10) do not require one to know the exact asymptotic eigenstates in the leads (as is the case with the "original" Landauer formulation relying on knowledge of the scattering basis of the wave functions defined within the asymptotic regions of the leads). This becomes *sine qua non* when computing the conductance of systems with complicated "leads," e.g., like in the case of atomic-size point contacts.[41]

Trace expressions like Eqs. (6) and (7) *do not* conserve the current. Therefore, the suggested strategy is to evaluate G_{ra} and G_{rr} by tracing over the states located on two planes inside the sample (or inside the leads), as well as over the whole sample (and see how close G_{ra} can get to G). Different types of conductors are chosen for this evaluation: weakly disordered with $W=2$ (e.g., $l \approx 9a$ at $E_F = 0$) and strongly disordered conductors with $W=7$ (for which unwarranted use of the Drude-Boltzmann formula would give[29] $l < a$). The exact computation of these traces is shown in the upper panels of Figs. 1 and 2 for a single-impurity configuration of $W=2$ [here G_{ra} is also computed by tracing over two planes deep inside the leads, which corresponds to integrating $\sigma(\mathbf{r},\mathbf{r}')$ over such cross section, as discussed above]. The lower panels of Figs. 1 and 2 plot disorder-averaged quantities over an ensemble of impurity configurations for disorder strength $W=7$. In both ways of tracing, the sum of two terms G_{ra} and G_{rr} gives the full expression for conductance $G(E_F)$, which have to cancel each other for $|E_F| > 6t$ in order to ensure vanishing of $G(E_F)$ when $t_L = t$ is chosen.
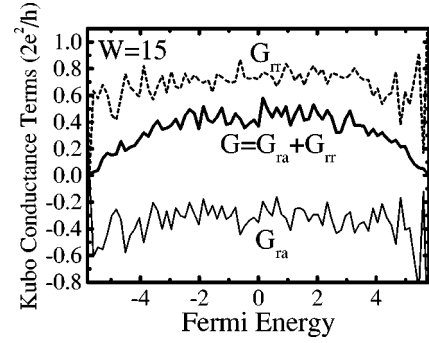

FIG. 4. Different terms in the Kubo formula $G = G_{ra} + G_{rr}$ for the two-probe quantum conductance of the finite-size conductor modeled on a 10^3 lattice with diagonal disorder $W=15$ (the whole band becomes localized at $W_c \simeq 16.5$). Respective traces in these expressions are performed over the site states inside the whole disordered sample and disorder averaged over 50 realizations.

The result for $W=7$ disorder belongs to the nonperturbative transport regime. It is interesting, therefore, to follow the behavior of G_{ra} and G_{rr} terms further throughout this regime, eventually reaching $W_c \simeq 16.5$ where the whole band becomes localized.[42] The generic LD transition point in 3D is beyond NLSM treatment inasmuch as it corresponds to a strong-coupling limit in field theoretical language. Furthermore, recent description[43] of Anderson localization in terms of an order parameter, obtained from a theory based on a local approximation, suggests that probing the instability of the delocalized phase through WL-type corrections might be a daunting road to reach the transition in 3D. Figure 4 shows that around W_c the conductance $G \sim 2e^2/h$ is mostly defined by the G_{rr} term—a situation completely opposite to the weak-disorder finding ($W=2$ in Figs. 1 and 2). Therefore, at some intermediate disorder $7 < W < 10$, within the nonperturbative transport regime, a transition occurs from $G_{ra} > G_{rr}$ to $G_{rr} > G_{ra}$, ending up eventually with a case $G_{ra} < 0 < G_{rr}$ around the LD critical point.

An inquisitive reader might have come up by now with the question as to what happens in the clean case. A
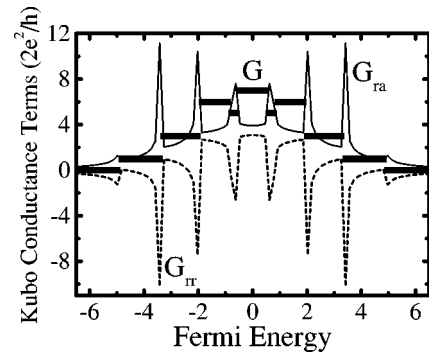

FIG. 5. Different terms in the Kubo formula $G = G_{ra} + G_{rr}$ for the two-probe quantum conductance of a clean finite-size conductor modeled on a 3^3 lattice ($\varepsilon_{\mathbf{m}} = 0$, $t = t_L = t_C = 1$). The conductance as a function of the Fermi energy changes in steps corresponding to the number of open conducting channels (defined by nine quantized transverse propagating modes).

mesoscopic ballistic sample attached to two leads has non-zero point contact conductance[38] of a purely geometrical origin since leads are widening into macroscopic reservoirs at infinity, where reflection occurs when the large number of conducting channels in the macroscopic reservoir matches the small number of channels in the lead.[44] Such point contact conductance is quantized[16] as a function of sample width[20] or Fermi energy,[21] which becomes conspicuous when the number of quantized transverse propagating modes (i.e., the sample cross section) is small enough. A clean ($\varepsilon_{\mathbf{m}} = 0$) $3 \times 3 \times 3$ toy sample illustrates conductance quantization in Fig. 5, as obtained from the two-probe Kubo formula for G. In this case, both terms G_{ra} and G_{rr} are contributing in a nontrivial fashion to a stepwise conductance.

What can be learned from these numbers is that G_{ra}, Eq. (6), can serve as a decent *approximation* to the exact Kubo formula for the quantum conductance G only in very weakly disordered conductors, where $l \gg a$. However, because of not conserving the current, the trace in G_{ra} has to be performed over the whole disordered region (which is an enormous computational effort and is therefore useless in real-space computational practice). The essential outcome of this exercise is the explicit quantification of the difference between G and G_{ra}. This and current conservation are important points to bear in mind when using the simplified expression G_{ra} in analytical derivations and arguments of the quantum transport theory.[3,16,20] Finally, the strong-disorder (nonperturbative) behavior of two different Green function terms, comprising the Kubo formula for quantum conductance, might provide a clue for the inadequacy of attempts to analyze a genuine Anderson transition in 3D by probing the instability of the metallic phase to weak-localization (perturbative) corrections.

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