Current-constraining variational approaches to quantum transport

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Presently, the main methods for describing a nonequilibrium charge-transporting steady state are based on time-evolving it from the initial zero-current situation. An alternative class of theories would give the statistical nonequilibrium density operator from principles of statistical mechanics, in a spirit close to Gibbs ensembles for equilibrium systems, leading to a variational principle for the nonequilibrium steady state. We discuss the existing attempts to achieve this using the maximum entropy principle based on constraining the average current. We show that the current-constrained theories result in a zero-induced drop in electrostatic potential, so that such ensembles cannot correspond to the time-evolved density matrix, unless left- and right-going scattering states are mutually incoherent.

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I. INTRODUCTION

The problem of charge transport through nanoscale objects became a very intensive area of research during the last few years. Numerical calculations reflect the rapidly advancing development of experimental techniques exploring typical characteristics of atomic wires or single-molecule junctions.[1,2] The most usual theoretical methods used to address these issues are either direct occupation of scattering states[3,4] or using the nonequilibrium Green's function formalism for steady-state (NEGF).[5,6] Both of these rely upon an assumption that the use of a ground-state density-functional theory gives the effective self-consistent potential. This assumption is now known not to be correct even though corrections to it might be relatively small, which is particularly true for systems with open channels.[7,8] The NEGF method makes use of semi-infinite reservoirs which demand further approximations to the effective potential if one is to be able to perform *ab initio* studies of the systems of interest, e.g., typically the electronic structure of the leads are taken as that of the leads in equilibrium. The errors included this way can be assessed and calculations for representative systems suggest them to be no more than a few percent.[9] A second source of discrepancies between the experimental and theoretical work comes from the ambiguity of the geometry of the molecular junction one employs. The most common choice is the ground state geometry. Even though several interesting results concerning nonequilibrium forces exist,[10,11] *ab initio* studies of current-distorted geometries are still absent.

Almost all of the above-mentioned development is based on time evolution as a means to obtain the nonequilibrium steady state,[12–14] although in most cases the time evolution is used only formally for the derivation of the formulas used within the NEGF formalism. The other alternative would be to use some sort of variational principle that would directly lead us to the nonequilibrium density matrix (or state). While it might be difficult to believe that such a principle would exist for a general dissipative system, its existence for the purposes of quantum transport is relatively easy to accept. At the level of a noninteracting or mean-field description of the electrons, it has been known for some time that such a variational principle exists,[15,16] and it can be extended formally to fully interacting electron systems, provided that there is a physical relaxation process that "washes out" initial correlations.[17] These are based on the search for a state with minimum energy, consistent with prescribed numbers of right- and of left-going electrons [hereafter referred to as the "left-right" scheme (LRS)] or prescribed average current (current constrained approaches). The LRS prescription is directly motivated by the Landauer-Büttiker formalism[18] developed for mesoscopic systems and can be generalized by maximizing the information entropy with constraints on the average energy (corresponding to the introduction of the temperature in equilibrium) and average numbers of left- and right-going particles. To remove the concept of single-particle orbitals from this approach, Frensley suggested to constrain the local Wigner distribution functions for electrons with positive and negative momenta in the left and right lead, respectively.[19] This has the advantage that it can be used also for interacting approaches as has been demonstrated recently by Delaney and Greer.[20] A different extension of the single-particle theory was presented by Hershfield,[17] who formally constructed a nonequilibrium steady-state density matrix using many-body field operators corresponding to generalizations of the scattering states.

As an alternative to the density constraint, several authors have suggested the total current as a means to keep the steady state out of equilibrium.[15,21–27] The current constraint, unlike the density constraint, immediately has a well-defined form even for interacting electrons. It was soon realized that the current-constrained density matrix corresponds to a situation different from that obtained within the LRS, although no clear consensus exists regarding what experimental situation it describes. It has been mentioned already in the work of Ng[15] that the theory should correspond to a constant current experiment (as opposed to constant voltage). However, this cannot be the only criterion, since the system of interest is very small and so the ability of the system to explore the whole Hilbert space of admissible density matrices should be

considered with care. The latter property is indeed at the center of the formulation employing constrained searches within the maximum entropy principle.[26,28] In this respect it is interesting to note recent work by Di Ventra and Todorov[27] who have formally considered a variational principle based on constraining the current for a quasi-steady-state of discharge of large but finite electrodes through a nanojunction. The steady-state-current constrained ensembles, which are the subject of the present paper, should correspond to a long-time and infinite-size limit of their considerations.

The various current-constraint formulations differ in some details. Ng[15] considers a treatment where the current operator is altered in such a way that it does not mix the right- and left-going scattering states. To achieve this one has to drop all the off-diagonal matrix elements of the current operator in the scattering states representation. This eventually leads to a theory that is similar to the LRS, but with the occupancies now depending on the current that the particular state carries, as well as its energy. The applied bias is determined from the difference in the local electrochemical potential between the left and right asymptotic regions which, strictly speaking, corresponds to the electrostatic drop around the sample. Heinonen and Johnson[21,22] consider only systems that are translationally invariant along the current flow. Under such circumstances the off-diagonal matrix elements of the current operator are absent by symmetry and the notion of applied bias is only formal. They determine the latter from the analogy with the scattering-states-occupation theory and the resulting *I-V* characteristics in the linear regime are identical to the LRS description. One should point out that this analogy fails as soon as one enters a strongly nonlinear *I-V* regime with, for example, a current flow through a resonant barrier.

In both of these treatments the effective Hamiltonian with the current constraint commutes with the physical Hamiltonian or, in other words, that the constrained density matrix is stationary. The approach developed by Kosov[23,24] departs from this point and instead constrains the current to be uniform throughout the system. As a result, the density matrix is not time independent which brings into question its relevance for the description of a steady state. The problem of the steady-state character of the density matrix obtained from a current-constrained search has been studied by the authors of this paper.[26] It has been found that the steady-state requirement *does* remove most of the off-diagonal matrix elements of the current operator, as is assumed by Ng. However, those off-diagonal elements between states with the same energy do *not* disappear, which leads to a density matrix different from that anticipated by Ng. The induced drop in the potential was found from the local neutrality conditions in the asymptotic regions, in a manner similar to that of Ng, and the paper additionally discussed the relation of the Lagrange multiplier A (that imposes the current constraint) to the applied bias voltage.

The aim of this paper is to present a clear relationship between the above-mentioned current-constraining schemes, as well as to discuss their limitations. We start by analyzing the role of the external applied bias within the formalism. This yields a link between the time-evolved and variational approaches, and gives a supportive argument for the form of the steady-state requirements implemented in our earlier work.[26] In Sec. III we address the induced drop in the electrostatic potential. Conversely to what has been claimed before we have found that unless we remove *all* of the off-diagonal elements of the current operator, the induced drop is exactly zero. This holds for the uniform-current approach, discussed in Sec. V, where all elements are retained[23] as well as for the approach (used in our previous study[35]) in which the current operator has off-diagonals only between equal-energy states. In Sec. IV we describe how many-body interactions of the electrons with the environment correct the previous results to a physically meaningful picture where nonzero drop in the potential is found and the agreement with the conventional approaches (NEGF, LRS) achieved within the linear response regime.

II. APPLIED EXTERNAL FIELD AND MAXIMUM ENTROPY

We describe the steady-state-current situation using the maximum entropy principle for the statistical density operator $\hat{\rho}$ (Ref. 28)

$$\delta\left\{-\mathrm{Tr}[\hat{\rho}\log(\hat{\rho})]-\sum_i \mathrm{Tr}\lambda_i[\hat{\rho}\hat{A}_i]\right\}=0, \tag{1}$$

where λ_i are Lagrange multipliers that guarantee chosen values A_i of the averages of chosen operators $\hat{A}_i$. That is, instead of following the specific time evolution caused by an applied external field, we assume that the final steady state is representable by the statistical density operator $\hat{\rho}$ that possesses the same current and/or induced drop in potential. While all of the existing schemes agree on using the total energy and total number of electrons as two of the constrained operators $\hat{A}_i$, the constraint that keeps the system out of equilibrium varies and is either the total current or the occupancies of right- and left-going scattering states.

In real-time evolution approaches, there are no nonequilibrium constraints or multipliers. Instead, the applied external field acts as a driving force for the current flow. The character of the external field seems to be a source of certain confusion in the community. Some authors use a ramplike external potential that has a finite slope between contacts[20,24] even within maximum entropy schemes, while some avoid its presence altogether.[15,17,21,22,26] On the other hand, in calculations based on the time evolution (scattering states, NEGF formalism), the role of the applied external field is frequently circumvented by the application of a difference in electrochemical potential between two initially isolated leads. The electrons are taken to be noninteracting while in the leads. This construction, however, leads to violation of local charge neutrality in the noninteracting regions as discussed elsewhere.[9] Neither does it clarify the relation between the total and induced electric field. Clearly, the problem with the applied external field can be tracked down to the fact that one tries to model the effect of the battery within the calculation.

The appropriate form of the external field is available from considerations originally made in the linear response regime.[29] To have a system infinite along the direction of

flow and characterized by a finite drop in external potential, ΔV, one needs to consider the large time limit of a field

$$E^{ext}(x,t) = \frac{\Delta V}{2vt}[\theta(x+vt) - \theta(x-vt)], \tag{2}$$

where $\theta(x)$ is the unit step function, x is the direction of current flow, and v is the desired speed of the front between the region with an applied field and that without field. This represents a situation that has a constant drop ΔV in the potential at all times t and, for sufficiently large $v \gg v_F$, it produces a uniform current even in the case of interacting electrons, i.e. the field is not screened out. The steady state is obtained in the $t \to \infty$ limit where the drop ΔV persists, but the external field in any finite part of system is zero. [e.g., $E^{ext}(x=0,t) = \Delta V/(vt) \to 0$]. The initial localization of the field-containing region leaves no long-time signature other than the steady current that flows, and associated changes in the electronic structure such as density or induced potential. The fact that the drop in *external* potential ΔV appears over an infinite distance may appear unfamiliar at first sight, but in most cases the main drop in the *total* potential will occur in a small region, owing to screening. For example, a nanoscale inhomogeneity that locally decreases the density of states at the Fermi energy will create a sharp drop in the induced potential—and therefore also the total potential—in the vicinity of the nanoscale region, even within a mean-field description.

The above considerations of the steady state show that the Hamiltonian *with zero applied field* must be used when constructing the density operator within the maximum entropy ansatz. Similarly, we believe that the use of a finite external field together with the maximum entropy prescription is simply incorrect, and its application in other calculations should be reconsidered. The *induced* field *will*, however, appear in the calculation as a consequence of the current constraint applied to the density matrix.

The second outcome of this observation concerns the steady-state character of the system. Once we accept that the Hamiltonian present is that without the applied field, the stationarity of the statistical density operator requires[26]

$$[\hat{\rho}, \hat{H}] = 0. \tag{3}$$

This identity has to be included when performing the constrained search for the operator $\hat{\rho}$. At the same time, it should be clear that this condition can be fulfilled only for a system infinite along the direction of the current flow. (The only exception is a system of perfect translational invariance and finite periodic boundary conditions. As this represents a very special and highly nongeneric case—an arbitrarily small perturbing potential spoils the perfect translational invariance and therefore the ability of the system to carry current—we will not be concerned with it in our further discussion.)

The condition (3) has been shown to follow also from a time-evolution point of view by Hershfield.[17] In this work it is also correctly pointed out that, as opposed to the equilibrium expectation value, nonequilibrium systems are characterized by an effective Hamiltonian that enters the statistical density operator, which is different from the true physical Hamiltonian characterizing the time evolution or time correlations in the system. This, as we will see, significantly complicates the formal development of the theory for interacting nonequilibrium steady-state systems.

III. THE INVARIANT CURRENT APPROACH AND THE INDUCED DROP IN THE POTENTIAL

In the invariant current approach the constraint that keeps the system out of equilibrium is chosen to be the current at a particular point x_0,

$$I(x_0) = \int d\vec{S} \cdot \mathrm{Tr}[\hat{\rho}\hat{j}(x_0,y,z)], \tag{4}$$

where $\hat{j}(x,y,z)$ is the operator of the current density at $\mathbf{r} = (x,y,z)$. As we have shown,[26] this requirement, together with the steady-state restriction (3), leads to the statistical operator

$$\hat{\rho} = \exp\{\Omega - \beta(\hat{H} - \mu\hat{N} - A\hat{I}^0)\}, \tag{5}$$

where the operator $\hat{I}^0$ is the invariant part of the current operator[26,30,31]

$$\hat{I}^0 = \lim_{T\to\infty} \frac{1}{2T}\int_{-T}^{T} \hat{I}(t)dt, \tag{6}$$

which is independent of the position of current measurement x_0. This arises from the fact that for a stationary density matrix the current fulfills the continuity equation $\nabla \cdot \hat{\mathbf{j}} = -\dot{n} = 0$. The time dependence of the operator $\hat{I}(t)$ is determined by the Hamiltonian of the system $\hat{H}$ which, similarly to the case of scattering field operators in Hershfield's work,[17] hinders the development of the theory for interacting electrons.

At the mean-field level of approximation, the one-particle density matrix can be used to obtain all required quantities. Instead of the many-body Hamiltonian we need to consider the effective one-particle Hamiltonian given by[36]

$$\hat{h} = -\tfrac{1}{2}\partial_x^2 + u(x) - \mu - AI^0(x), \tag{7}$$

where $u(x)$ is the self-consistent potential approaching constant values in the right- and left-asymptotic limits (i.e., an asymptotically homogeneous system), μ chemical potential, A a Lagrange multiplier belonging to the current constraint and I^0 the invariant current operator. Even though we eventually obtain the one-particle density matrix that closely resembles the usual local Fermi distribution, its derivation is nontrivial. The problem arises from the fact that our system cannot, strictly speaking, be obtained as a limit of a finite one. First, the finite drop in the potential $\Delta u = u(\infty) - u(-\infty)$, makes it impossible to consider periodic boundary conditions, and, second, the existence of a nonzero current flow hinders the construction of hard walls placed at finite, but large distances at right and left, as used by Adawi.[32] Similarly, the use of periodic boundary conditions, that implicitly appear in some current-constraint-based treatments,[15,21,22] is not consistent with the possible existence of an overall drop in the electrostatic potential and the nonzero current. For

these reasons we give its detailed derivation in Appendix A. The resulting one-particle density matrix is

$$n(x,x') = \sum_{\alpha} \int dE \frac{\chi_{E,\alpha}(x)\chi^{*}_{E,\alpha}(x')}{e^{\beta(\tilde{E}_{\alpha}(E)-\mu)}+1}, \tag{8}$$

where $\chi_{E,\alpha}(x)$ are energy-normalized states that diagonalize the Hamiltonian (7) and $\tilde{E}_{\alpha}(E)$ are the corresponding eigenvalues. The latter can be expressed in the basis of scattering states of the physical Hamiltonian [i.e., without the term containing the current operator in Eq. (7)]

$$\chi_{E,\alpha}(x) = \sum_{\nu} \phi_{E,\nu}(x) U_{\nu,\alpha}(E), \tag{9}$$

where $\phi_{E,\nu}(x)$, $\nu = R,L$ represent right- or left-going scattering states at the energy E given asymptotically as

$$\phi_{E,R}(x \gg 0) = \frac{1}{\sqrt{2\pi k}} t e^{iqx}, \tag{10}$$

$$\phi_{E,L}(x \ll 0) = \frac{1}{\sqrt{2\pi k}} \tilde{t} e^{-ikx}, \tag{11}$$

where $k = \sqrt{2E}$ and $q = \sqrt{2(E+\Delta u)}$ are the wave vectors on the far left and far right, respectively, and t and $\tilde{t}$ are transmission amplitudes for right-going and left-going electrons, respectively. (t and $\tilde{t}$ depend on the energy but we will not write this dependence explicitly.) We note that the states $\chi_{E,\alpha}$ can be labeled with the energy because the effective Hamiltonian commutes with the physical one, as required by the stationarity condition (3). From this and a glance at Eq. (7) it follows that the states $\chi_{E,\alpha}$ are simultaneously eigenstates of the invariant current operator I^0. Therefore the second index differentiates between energy-degenerate states which, in the simplest case of a single 1D channel considered here, attains two different values, "+" and "−," depending on the sign of the invariant current eigenvalue of the respective state. In Appendix B we show that the states $\chi_{E,+}$ and $\chi_{E,-}$ transform one into another under the time reversal T,

$$T\chi_{E,+} = \chi^{*}_{E,+} = e^{i\xi}\chi_{E,-}, \tag{12}$$

where ξ is an unspecified, but well defined phase. The above relation has an important consequence for the induced change in the density in the linear regime, as we will discuss below.

We have already indicated that the scattering-states representation plays a fundamental role not only in the LRS approach but also in the current-constraint schemes. It is therefore useful to express the current operator in the scattering states representation[33]

$$2\pi \frac{dI_{\nu,\eta}(x \ll 0)}{dE} = \delta_{\nu,1}\delta_{\eta,1} - S^{\dagger}_{\nu,1}S_{1,\eta} = \begin{bmatrix} 1-|r|^2 & -r^{*}\tilde{t} \\ -r\tilde{t}^{*} & -\frac{k}{q}|\tilde{t}|^2 \end{bmatrix}, \tag{13}$$

$$2\pi \frac{dI_{\nu,\eta}(x \gg 0)}{dE} = -\delta_{\nu,2}\delta_{\eta,2} + S^{\dagger}_{\nu,2}S_{2,\eta} = 2\pi \frac{dI_{\nu,\eta}(x \ll 0)}{dE}, \tag{14}$$

where $S_{\nu,\eta}$ is the scattering matrix

$$S_{\nu,\eta} = \begin{bmatrix} r & \tilde{t} \\ t & \tilde{r} \end{bmatrix} \tag{15}$$

and the last equality in Eq. (14) follows from the unitarity of $S_{\nu,\eta}$ (current conservation) and t,r and $\tilde{t},\tilde{r}$ are the transmission and reflection amplitudes for right- and left-going electrons. Similarly to the latter, we do not write explicitly the energy dependence of the S matrix or the current operator matrix. The current matrix elements are differentials with respect to energy due to the energy normalization of the scattering states; the element corresponds to the current carried by an electron occupying states in the energy interval $(E, E+dE)$. Since the invariant current operator I^0 in Eq. (7) is related to the matrix of the current operator multiplied by a delta-function of energy (see Appendix A),

$$I^0(E,\alpha;E',\beta) \times A = \frac{dI_{\alpha,\beta}}{dE}\delta(E-E') \times \tilde{A}, \tag{16}$$

where $\tilde{A}$ is a renormalized Lagrange multiplier $\tilde{A} = \lim_{T\to\infty} \pi A/T$ attaining finite values for constraining the current to finite nonzero values, the states $\chi_{E,\alpha}(x)$ automatically diagonalize the kinetic and potential energy terms in Eq. (7). To diagonalize the complete effective Hamiltonian they need to diagonalize also the current operator which is given by Eq. (13). The unitary transform that achieves this has been found before[26]

$$U_{\nu\alpha} = \begin{bmatrix} \frac{r^{*}\tilde{t}/|t|}{\sqrt{2(1-|t|)}} & \frac{r^{*}\tilde{t}/|t|}{\sqrt{2(1+|t|)}} \\ \frac{|t|-1}{\sqrt{2(1-|t|)}} & \frac{|t|+1}{\sqrt{2(1+|t|)}} \end{bmatrix} \tag{17}$$

with the corresponding effective eigenvalues

$$\tilde{E}_{\alpha}(E) = E \pm \tilde{A}|t|. \tag{18}$$

The calculation of the current is then straightforward using the one-particle density matrix,

$$\langle I(x) \rangle = \sum_{\alpha,\nu,\eta} \int dE \frac{1}{e^{\beta[\tilde{E}_{\alpha}(E)-\mu]}+1} U^{\dagger}_{\alpha,\nu} \frac{dI_{\nu,\eta}(x)}{dE} U_{\eta,\alpha}. \tag{19}$$

Using this expression we find the dependence of the current on the renormalized Lagrange multiplier $\tilde{A}$.

For comparison with other approaches as well as experiments, we also need the dependence of the current on the drop in the electrostatic potential, Δu, which can be obtained from the induced change in the density $\delta n(x)$ via the expression

$$u(x) = \int v(x,x')\delta n(x')dx',$$

$$\Delta u = u(+\infty) - u(-\infty), \tag{20}$$

where $v(x,x')$ is an appropriate effective electron-electron interaction. Alternatively, Δu can be obtained from the local neutrality conditions in the right and left electrodes[9] for the self-consistently determined scattering matrix (hence the link to the resistivity dipoles based formula). The local neutrality conditions demand

$$-n(x \ll 0) + n_B = 0, \tag{21}$$

$$-n(x \gg 0) + n_B = 0, \tag{22}$$

where n_B is the positive charge density of the background, assumed to be the same in both electrodes for simplicity. Subtracting these two we get a single condition[37]

$$\Delta n = n(x \ll 0) - n(x \gg 0) = 0. \tag{23}$$

This identity alone can be used to determine the drop in the potential Δu, for given values of $\tilde{A}$ and μ. The density in the asymptotic regions is obtained in a way similar to the total current: we first find the expressions for the matrix of the density in the asymptotic regions within the scattering states representation

$$\frac{dn_{\nu\eta}(x \ll 0)}{dE} = \frac{1}{2\pi k}\delta_{\nu,1}\delta_{\eta,1} + \frac{1}{2\pi k}S^{\dagger}_{\nu,1}S_{1,\eta} = \frac{1}{\pi k}\delta_{\nu,1}\delta_{\eta,1} - \frac{1}{k}\frac{dI_{\nu\eta}(x \ll 0)}{dE}, \tag{24}$$

$$\frac{dn_{\nu\eta}(x \gg 0)}{dE} = \frac{1}{2\pi q}\delta_{\nu,2}\delta_{\eta,2} + \frac{1}{2\pi q}S^{\dagger}_{\nu,2}S_{2,\eta} = \frac{1}{\pi q}\delta_{\nu,2}\delta_{\eta,2} + \frac{1}{q}\frac{dI_{\nu\eta}(x \gg 0)}{dE}. \tag{25}$$

Second, we express the local neutrality condition (23) using the density matrix

$$\sum_{\alpha,\nu,\eta}\int dE \frac{1}{e^{\beta(\tilde{E}_{\alpha}(E)-\mu)}+1}U^{\dagger}_{\alpha,\nu} \times \left[\frac{dn_{\nu,\eta}(x \ll 0)}{dE} - \frac{dn_{\nu,\eta}(x \gg 0)}{dE}\right]U_{\eta,\alpha} = 0. \tag{26}$$

To obtain algebraic results we need to restrict our treatment to the $\beta \to \infty$ limit (corresponding to the density matrix with the minimal energy for given constraints). Under these circumstances the effective Fermi distribution takes the form

$$\frac{1}{e^{\beta(\tilde{E}_{\alpha}(E)-\mu)}+1} \approx \delta_{\alpha,1}\theta(\mu - E + \tilde{A}|t(E)|) + \delta_{\alpha,2}\theta(\mu - E - \tilde{A}|t(E)|), \tag{27}$$

where the two step functions $\theta(\,)$ correspond to the positive and negative eigenvalues in Eq. (18). Assuming $\tilde{A} > 0$, we see that starting from $E > \mu_2 = \mu - \tilde{A}|t(\mu_2)|$ and up to $E < \mu_1 = \mu + \tilde{A}|t(\mu_1)|$, only one of the two degenerate states $\chi_{E,\alpha}$ will be occupied.[38]

For $E < \mu_2$ the contributions to the density clearly cannot depend on the unitary rotation between the scattering states and we therefore have

$$\sum_{\alpha}\frac{dn_{\alpha,\alpha}}{dE}(x \ll 0) = \sum_{\alpha,\nu,\eta}U^{\dagger}_{\alpha,\nu}\frac{dn_{\nu,\eta}}{dE}(x \ll 0)U_{\eta,\alpha} = \frac{1}{\pi k}, \tag{28}$$

$$\sum_{\alpha}\frac{dn_{\alpha,\alpha}}{dE}(x \gg 0) = \frac{1}{\pi q}. \tag{29}$$

The contribution from the singly occupied state $\chi_{E,\alpha=1}(x)$ we find from Eqs. (24), (25), and (17) with a surprisingly simple result

$$\frac{dn_{11}}{dE}(x \ll 0) = \sum_{\nu,\eta}U^{\dagger}_{1,\nu}\frac{dn_{\nu,\eta}}{dE}(x \ll 0)U_{\eta,1} = \frac{1}{2\pi k}, \tag{30}$$

$$\frac{dn_{11}}{dE}(x \gg 0) = \frac{1}{2\pi q}. \tag{31}$$

Finally combining Eqs. (27), (29), (28), (30), and (31) in Eq. (26) we get

$$\int_0^{\mu_2}\frac{dE}{\pi k} + \int_{\mu_2}^{\mu_1}\frac{dE}{2\pi k} - \int_{-\Delta u}^{\mu_2}\frac{dE}{\pi q} - \int_{\mu_2}^{\mu_1}\frac{dE}{2\pi q} = 0. \tag{32}$$

The last equation can be satisfied only for $\Delta u = 0$. This means that the invariant-current scheme with the off-diagonal elements at the same energy retained leads to *no induced potential drop* and therefore its applicability to common nanocontacts is doubtful, even in a constant-current experiment. We would like to note that zero drop in the total potential is not a contradiction with the fact that the system carries a finite nonzero current: the current is maintained by nonzero value of the parameter $\tilde{A}$ or, equivalently, a nonzero value of the difference $\mu_1 - \mu_2$.

Qualitatively, the result $\Delta u = 0$ is a consequence of the fact that the contribution to the density per energy of each doubly degenerate state $\chi_{E,\alpha}$, $dn_{\alpha,\alpha}/dE$, is almost the same[39] far right and far left [see Eqs. (30) and (31)]. If we assume that the right electrode, having the same background charge density as the left one, has the bottom of its local density of states at $E = -\Delta u$, below that of the left electrode ($E = 0$), occupying this portion of the energy spectrum ($E < 0$) will partially compensate for the background charge in the right electrode. Once the states below the bottom of the left electrode are filled, adding each electron into next state $\chi_{E,\alpha}$ will contribute in both electrodes almost equally so that when attempting to compensate for the background charge of the left electrode we will inevitably overload the right electrode or, when neutralizing the right electrode there will not yet be enough electronic charge in the left one. [We would like to stress that the above reached conclusions are valid for $\beta \to \infty$ limit, finite $\tilde{A}$ and a regime, in which the equations for μ_1 and μ_2 have a unique solution. The latter fails to be fulfilled if either μ_1 or μ_2 approaches a resonant energy level of the potential $u(x)$.]

An even more surprising result appears in the linear response regime, i.e., when $AI^0 \ll \mu$. Under these circumstances the induced change in the density $\delta n(x)$,

$$\delta n(x) = n(x,x)|_{\tilde{A}} - n(x,x)|_{\tilde{A}=0},$$

where $n(x,x)|_{\tilde{A}}$ is the diagonal of the density matrix given in Eq. (8) for a given (small) value of the renormalized Lagrange multiplier $\tilde{A}$, is simply given by

$$\delta n(x) = 2\tilde{A}|t(\mu)|(|\chi_+(x)|^2 - |\chi_-(x)|^2) + O(|\tilde{A}|^2). \quad (33)$$

Using the time-reversal character of the states $\chi_{E,\alpha}$, Eq. (12), we immediately obtain that $\delta n(x) = O(|\tilde{A}|^2)$, i.e., there is no change of the density in the linear regime. Using this result in the formula for the induced drop, Eq. (20), we once again confirm the above obtained result (valid even for finite $\tilde{A}$) of the zero-induced drop in the electrostatic potential.

IV. THE INVARIANT CURRENT APPROACH WITH DECOHERENCE

In the preceding section we have assumed a full coherence of the electronic system—an assumption that can be hardly justified for junctions with low transmission. In this section we show that it was precisely this assumption that led to the unphysical results and that accounting for the interactions of the leads with the environment removes these problems. As we will show below, this results in removing the off-diagonals of the invariant current operator. This makes the density matrix (8) identical to that given by Ng.[15] The elimination of the off-diagonals can be made physically plausible from the assumption of phase independence between the right- and left-going scattering states. Namely, if we ascribe an independent fluctuating phase $e^{i\theta_\nu}$ to each of these two, the off-diagonal matrix elements of the one-particle density matrix, Eq. (8), are easily seen to be averaged to zero. The effect of the coupling to the environment is to suppress, through averaging over a fluctuating phase, any mixing of left- and right-going states in the pure states that are summed in the density matrix. In effect, these pure states are constrained to be either left- or right-going. This means that the off-diagonal elements of the current operator no longer play any role in the determination of the steady-state density matrix.

To recast the above considerations into a more formal language we need to include a description of the effect of the environment in the Green's-function-based derivation of the one-particle density matrix given in Appendix A. The Green's function, that directly leads to the one-particle density matrix, is defined in terms of the time-ordered product of the field operators,

$$G(2,1) = -\mathrm{Tr}[\hat{\rho}T\{\psi(2)\psi^\dagger(1)\}], \quad (34)$$

where $\hat{\rho}$ is the many-body density matrix that specifies occupations of the states of the whole system, i.e., the degrees of freedom of the environment that cause the above discussed fluctuating phases. Rewriting the Green's function in terms of creation and annihilation operators of electrons in the scattering states,

$$G(2,1) = -\int dE dE' \sum_{\nu,\eta} \phi_{E,\nu}(x)\phi^*_{E',\eta}(x') \times \mathrm{Tr}[\hat{\rho}T\{c_{E,\nu}(t_2)c^\dagger_{E',\eta}(t_1)\}], \quad (35)$$

we observe that the Green's function will have *only* the diagonal elements with respect to the $\nu, \eta = R/L$ index, i.e.,

$$\mathrm{Tr}[\hat{\rho}T\{c_{E,\nu}(t_2)c^\dagger_{E',\eta}(t_1)\}] \approx \mathrm{Tr}\left[\int \frac{d\theta_\nu d\theta_\eta}{4\pi^2}\hat{\rho}_e e^{i\theta_\nu}e^{-i\theta_\eta}T\{c_{E,\nu}(t_2)c^\dagger_{E',\eta}(t_1)\}\right] \sim \delta_{\nu,\eta}, \quad (36)$$

where $\hat{\rho}_e$ is a many-electron density operator already *without* the environment's degrees of freedom which were effectively taken into account via averaging over the phases of the right- and left-going scattering states. From this it follows that the equation of motion for this Green's function, Eq. (A8), is already in a diagonal form and so is the one-particle density matrix $n(x,x')$, Eq. (17).

Anticipating the sources of decoherence and therefore the irrelevance of the invariant current operator's off-diagonal elements, we can proceed rather straightforwardly in a derivation of Ng's[15] as well as our former results[26] for the theory with decoupled right- and left-going states. Since the current matrix (13) is effectively in a diagonal form, we can obtain the results considering the transform $U_{\nu,\alpha} = \delta_{\nu,\alpha}$, so that the states $\chi_{E,\alpha}(x)$, entering the one-body density matrix (8), are directly the scattering states. The effective eigenvalues prescribing the occupations are then given by

$$\tilde{E}_\alpha(E) = E \pm \tilde{A}|t(E)|^2. \quad (37)$$

What comes as an essential difference, as compared to the case when the decoherence is not accounted for, is that the contribution to the density from the singly occupied states now gives

$$\frac{dn_{11}}{dE}(x \ll 0) = \frac{2 - |t(E)|^2}{2\pi k}, \quad (38)$$

$$\frac{dn_{11}}{dE}(x \gg 0) = \frac{|t(E)|^2}{2\pi q}, \quad (39)$$

as can be easily seen by inspection of the expressions (24), (25), and (13). Clearly, the contributions to the local densities far right and far left are now significantly different and therefore the qualitative argument for zero induced drop in the potential does not apply. Using expressions (38) and (39) in the local neutrality condition (23) eventually leads to the linear response result

$$\Delta u = 2\tilde{A}|t(\mu)|^2|r(\mu)|^2. \quad (40)$$

Using Eqs. (19), (27), and (13) we obtain the current in the linear response

$$\langle I\rangle = 2\tilde{A}|t(\mu)|^2\frac{|t(\mu)|^2}{2\pi}, \tag{41}$$

and therefore combining the last two expressions we arrive at the well known result[18]

$$\frac{I}{\Delta u} = \frac{1}{2\pi}\frac{|t(\mu)|^2}{|r(\mu)|^2}, \tag{42}$$

for the so called 4-point conductance, a result already mentioned also within current constraining schemes[15,26] and in agreement with the LRS and therefore it is also compatible with the linear regime of the Landauer-Büttiker formalism.

To summarize this section, incorporating a decoherence caused by many-body interactions, the invariant current approach does lead to a nonzero induced drop and the resulting conductance is identical to that obtained within NEGF formalism as well as the LRS. We should stress that the way we have incorporated the decoherence contains assumptions regarding the coupling of the states to the environment and therefore cannot be regarded as a truly *ab initio* approach. The second important outcome is that formulating the maximum-entropy current-constrained scheme that starts at the noninteracting or mean-field self-consistent field level will not give physically meaningful results.

V. THE UNIFORM-CURRENT THEORY

In the uniform-current theory[23–25] one takes the constraint to make the current uniform throughout the system

$$I = I(x) = \langle\hat{j}(x)\rangle. \tag{43}$$

This is achieved by introducing a continuous Lagrange multiplier $\mathcal{A}(x)$ and the corresponding DM takes the form

$$\hat{\rho}^{UC} = \exp\left\{\Omega^{UC} - \beta\left(\hat{H} - \mu\hat{N} - \int dx\mathcal{A}(x)\hat{I}(x)\right)\right\}. \tag{44}$$

The function $\mathcal{A}(x)$ has to be found such that the constraint (43) holds. The essential difference from the invariant-current scheme is the fact that this ansatz results in a density matrix which evidently does not commute with the physical Hamiltonian

$$[\hat{\rho}^{UC},\hat{H}] \neq 0. \tag{45}$$

As a consequence, even though the current is uniform at some instant (and therefore from the continuity equation the density is momentarily stationary), it will in general change at later times together with many other averages computed using the $\hat{\rho}^{UC}$.

Apart from this objection, one can show that the scheme is equivalent to a equilibrium-like calculation with some effective potential, using a gauge transformation. Similarly to the invariant current theory, it emerges that the induced drop in electrostatic potential is zero. We will demonstrate this at the mean-field level of approximation only, even though it presents no complication in this case to prove it for fully interacting electrons as well. We first reformulate the many-particle problem of the full density matrix $\hat{\rho}^{UC}$ into that of one-body density matrix, in a way completely analogous to the previous section and the formalism given in Appendix A. Eventually we will be concerned with the mean-field single-particle Hamiltonian of the form

$$\hat{h} = -\tfrac{1}{2}\partial_x^2 + u(x) + \int d^3x'\mathcal{A}(x')\hat{I}(x')$$
$$= \tfrac{1}{2}[-i\partial_x + \mathcal{A}(x)]^2 + u(x) - \tfrac{1}{2}\mathcal{A}^2(x), \tag{46}$$

where $\mathcal{A}(r)$ is the same Lagrange multiplier as used in the many-particle density matrix, the current operator is

$$\hat{I}_x(x') = -\frac{i}{2}[\partial_x\delta(x-x') + \delta(x-x')\partial_x], \tag{47}$$

where the subscript x reminds us that the operator operates on functions of x. In this way the nonequilibrium problem has been transformed into a complex (so that current flow is possible in an effectively equilibrium-like system) but Hermitian eigenvalue problem on the whole space $x\in(-\infty,\infty)$ (so that the eigenstates form a continuum)

$$\hat{h}\chi_{E,\alpha}(x) = E\chi_{E,\alpha}(x). \tag{48}$$

The final one-particle density matrix is given by analogy with the previous section by the expression

$$n(x,x') = \sum_\alpha \int dE\frac{\chi_{E,\alpha}(x)\chi^*_{E,\alpha}(x')}{e^{\beta(E-\mu)}+1}. \tag{49}$$

However, the complex character of the problem can be removed by a simple gauge transformation

$$\chi_{E,\alpha}(x) = \exp\left(-i\int^x \mathcal{A}(x')dx'\right)\phi_{E,\alpha}(x), \tag{50}$$

where the transformed states $\phi_{E,\alpha}$ are eigenstates of a real Hamiltonian

$$\hat{h}' = -\tfrac{1}{2}\partial_x^2 + u(x) - \tfrac{1}{2}\mathcal{A}^2(x). \tag{51}$$

From this follows that the one-body density matrix

$$n(x,x') = \sum_\alpha \int dE\exp\left(-i\int^x \mathcal{A}(\xi)d\xi\right)\frac{\phi_{E,\alpha}(x)\phi^*_{E,\alpha}(x')}{e^{\beta(E-\mu)}+1}$$
$$\times\exp\left(i\int^{x'} \mathcal{A}(\xi)d\xi\right), \tag{52}$$

gives nonzero current only through the gauge factors. The current can be therefore easily evaluated to give

$$\langle I(x_0)\rangle = \int dxdx'\,\delta(x-x')\hat{I}_x(x_0)n(x,x') = \mathcal{A}(x_0)n(x_0), \tag{53}$$

where $n(x)$ is the electronic density. We can now fulfill the requirement of uniformity of the current by giving the Lagrange multiplier as

$$\mathcal{A}(x) = \frac{I}{n(x)}, \tag{54}$$

which makes the similar results of the previous work by Kosov[24] completely general (the same result holds for interacting electrons since the gauge transform argument does not depend on the interactions). Using the result (54) within the effective Hamiltonian (51) gives a simple closed set of equations to be solved.

Finally we turn to the analysis of the induced drop in the electrostatic potential which, similarly to the case of the invariant current theory, is identically zero. To show this we note that the self-consistent potential $u(x)$ used to determine the wave functions and therefore, via Eq. (52), the density, does not have any finite drop as it corresponds to a fictitious equilibrium system [the effective Fermi function in Eq. (52) depends only on the energy of the single-particle wave function $\phi_{E,\alpha}(x)$] for which the drop must be clearly zero. This observation is not affected by the presence of the last term in the effective Hamiltonian (51) since in the case of identical electrodes

$$\mathcal{A}(x \to \infty) - \mathcal{A}(x \to -\infty) = I(1/n_B - 1/n_B) = 0, \tag{55}$$

and the contribution so the drop in potential is zero.

VI. CONCLUSIONS

In conclusion, we have shown how the maximum-entropy formalism can be applied for nonequilibrium steady states within the framework of the single-particle approximation. We have presented three different approaches within a common formalism: (1) the invariant-current constraint, (2) the invariant-current constraint without the off-diagonals, and (3) the uniform-current constraint scheme. For these we have rigorously derived the one-particle density matrix for an infinite system that cannot be realized as a limit of a finite system. Subsequently we have obtained the expression for the electrostatic drop between electrodes within the linear response regime. We have shown that (1) and (3) give a zero-induced drop in electrostatic potentials which is not compatible with actual current-carrying situations in nanojunctions. In case (2) we have shown that by removing the off-diagonal elements of the current operator, the induced drop is nonzero and in fact, the results in the linear response are identical to the LRS. We can view the three different schemes analyzed in the two last sections from a more general perspective. They represent a variational prescription for the search of the nonequilibrium state with a given average of total current. The key difference between them is the part of a current operator that is being used for the constraint. The uniform-current theory takes the whole, unmodified current operator; the invariant-current scheme (through the stationarity requirement) removes the off-diagonals between states of different energy; and finally there is the form of invariant-current theory in which the off-diagonal elements within the scattering states basis set representation are removed by decoherence. Interestingly, only the last gives a electronic density which results in a nonzero induced drop in the potential. This observation raises a question whether there is something inherently wrong with demanding the current to be fixed. The theory with no off-diagonal elements of the current operator shows that the explanation for the problems with the current-constraining schemes arises from the fact that many-particle interactions or a certain source of decoherence is essential for the density matrix to give physically meaningful results.

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APPENDIX A: DERIVATION OF THE ONE-PARTICLE DENSITY MATRIX

To derive the form of the one-particle density matrix we first define an auxiliary Green's function, in a close analogy with the Matsubara technique,[34]

$$G(2,1) = -\mathrm{Tr}[\hat{\rho}\mathrm{T}\{\psi(2), \psi^{\dagger}(1)\}], \tag{A1}$$

$$\psi^{\dagger}(1) = e^{\hat{K}\tau_1}\psi^{\dagger}(x_1)e^{-\hat{K}\tau_1}, \psi(2) = e^{\hat{K}\tau_2}\psi(x_2)e^{-\hat{K}\tau_2}, \tag{A2}$$

$$\hat{K} = \hat{H} - \mu\hat{N} - A\hat{I}^0, \tag{A3}$$

where $\psi^{\dagger}(x)$ and $\psi(x)$ are the field operators for electrons. The fictitious time dynamics is given by the effective many-particle Hamiltonian $\hat{K}$, such that one can employ the similarity between the unitary time evolution operator and the density matrix $\hat{\rho}$ Eq. (5). The Green's function defined in this way satisfies the equation of motion

$$\left[-\tfrac{1}{2}\partial_x^2 + u(x) - \mu - AI^0(x) + \partial_\tau\right]G(x,x') = -\delta(x-x'), \tag{A4}$$

with the fermionic boundary condition

$$G(\tau = 0, \tau') = -G(\tau = \beta, \tau'). \tag{A5}$$

We note that while the many-body effective Hamiltonian $\hat{K}$ in (A3) is infinite and therefore just a formal expression, the one-body Hamiltonian present in the equation of motion for the Green's function (A4) is finite, for it represents energy *per* particle. The scattering states $\phi_{E,\nu}(x)$ Eqs. (10) and (11) diagonalize the Hamiltonian $-\frac{1}{2}\partial_x^2 + u(x)$ and therefore leave the elements of I^0 in a block-diagonal (diagonal with respect to the energy) form given by[26]

$$I^0_{\nu,\eta}(E,E') \times A = \lim_{T\to\infty}\frac{1}{2T}\int_{-T}^{T} dt\langle\phi_{E,\nu}|\hat{I}(x,t)|\phi_{E,\eta}\rangle \times A \tag{A6}$$

$$= \frac{dI_{\nu,\eta}}{dE}(x \ll 0) \times \delta(E-E') \times \tilde{A}, \tag{A7}$$

where we have used the renormalization of the current-related thermodynamic parameter A into $\tilde{A}=\lim_{T\to\infty}\pi A/T$. The matrix $dI_{\nu,\eta}/dE$ is the matrix of current operator at energy E given by Eq. (13). The equation of motion for $G(\tau)$ in the scattering-states representation now takes the form

$$\sum_{\nu'}\left[(E-\mu)\delta_{\nu,\nu'} - \tilde{A}\frac{dI_{\nu,\nu'}}{dE} + \partial_\tau\right] G^{\nu',\eta}_{E,E''}(\tau,\tau') = -\delta(\tau-\tau')\delta(E-E'')\delta_{\nu,\eta}, \tag{A8}$$

where

$$G^{\nu,\eta}_{E,E'}(\tau,\tau') = \langle \phi_{E,\nu}|G(x,x')|\phi_{E',\eta}\rangle. \tag{A9}$$

It is now clear that to solve (A8) we finally need to diagonalize the current matrix, i.e., employ the unitary transformation $U_{\alpha,\nu}$ discussed in Sec. III. The equation of motion after this transform takes a simple form

$$(\tilde{E}_\alpha - \partial_\tau)G^{\alpha,\beta}_{E,E'}(\tau) = -\delta(\tau-\tau')\delta_{\alpha,\beta}\delta(E-E'). \tag{A10}$$

We will drop the energy E,E' and state α,β indices for a moment since all the following manipulations are diagonal with respect to these. Regarding the time, the Green's function must obey the fermionic boundary condition

$$G(0) = -G(-\beta). \tag{A11}$$

The general solution of Eq. (A10) is clearly

$$G = \begin{cases} Ce^{-\tilde{E}(\tau+\beta)}, & -\beta < \tau < \tau' \\ -Ce^{-\tilde{E}\tau}, & \tau' < \tau < 0. \end{cases} \tag{A12}$$

Integrating the equation of motion over $\int_{\tau'-\delta}^{\tau'+\delta}$ we see that $G(\tau)$ must have a unit step discontinuity at $\tau=\tau'$ so that we can fix the constant C

$$Ce^{-\tilde{E}(\tau'+\beta)} - (-Ce^{-\tilde{E}\tau'}) = 1 \tag{A13}$$

and therefore

$$C = \frac{e^{\tilde{E}\tau'}}{1+e^{-\tilde{E}\beta}}. \tag{A14}$$

The density matrix is then given by

$$G(\tau,\tau') = \frac{e^{\tilde{E}\tau'}}{1+e^{-\tilde{E}}} \times \begin{cases} e^{-\tilde{E}(\tau+\beta)}, & \beta < \tau < \tau' \\ -e^{-\tilde{E}\tau}, & \tau' < \tau < 0 \end{cases} \tag{A15}$$

and the density matrix through the prescription is

$$\hat{n} = G(\tau = 0^-, 0) = \frac{e^{-\tilde{E}0^-}}{e^{\beta\tilde{E}}+1}. \tag{A16}$$

Restoring all the indices we finally have

$$n(x,x') = G(x,\tau=0^-;x',\tau'=0) = \sum_\alpha \int dE \frac{\chi_{E,\alpha}(x)\chi^*_{E,\alpha}(x')}{e^{\beta\tilde{E}_\alpha(E)}+1}, \tag{A17}$$

which is the result (8) given in Sec. III.

The above given derivation also shows that our approach does not depend on the choice of the normalization. If we had chosen the scattering states normalized to a δ function of k instead of E, the current matrix elements (13) would have to be multiplied by k. However, the δ function of energy in (13) is unchanged, since it comes from the general considerations of stationarity of the ensemble[26] so that we have $k\delta(E-E')=\delta(k-k')$. Using this in the equation of motion for G see, that the final result is the same, i.e., it is again the matrix elements of current in the energy-normalized states that appear in the effective dispersion relation.

APPENDIX B: TIME-REVERSAL SYMMETRY AND THE MAXIMUM ENTROPY STATES

In this appendix we show that the states $\chi_+(x)$ and $\chi_-(x)$ are related by the time-reversal symmetry

$$T\chi_+(x) = \chi^*_+(x) = e^{i\phi}\chi_-(x). \tag{B1}$$

Let $\hat{h}^0=\hat{h}+AI^0$ be the physical one-particle Hamiltonian in Eq. (7). Next, let $|\chi_{+/-}\rangle$ be the single-particle states that diagonalize both $\hat{h}^0$ and I^0. We will use T for the time reversal operator which is simply a complex conjugation. We have

$$\hat{h}^0|\chi_+\rangle = e|\chi_+\rangle, \tag{B2}$$

$$\hat{h}^0 T|\chi_+\rangle = eT|\chi_+\rangle \quad \text{since } [H^0,T]=0, \tag{B3}$$

$$I^0|\chi_+\rangle = +i|\chi_+\rangle, \tag{B4}$$

$$I^0 T|\chi_+\rangle = -iT|\chi_+\rangle \quad \text{since } TI^0 = -I^0T. \tag{B5}$$

The last property of the current operator is true for representation of operators and wave functions in a real space, where complex conjugation of the current operator changes its sign. Identical statements hold for the left-current-carrying maximum-entropy state $|\chi_-\rangle$ only with a reversed sign of the current eigenvalue i.

We know that $|\chi_+\rangle$ and $|\chi_-\rangle$ are degenerate eigenstates with an eigenvalue e. From Eq. (B3) we see that $T|\chi_+\rangle$ is also a state degenerate with them, and from Eq. (B5) that it has the same current eigenvalue as $|\chi_-\rangle$. Since this exhausts the possible degeneracy (twofold in 1D), the only possibility is that

$$T|\chi_+\rangle = e^{i\phi}|\chi_-\rangle,$$

where ϕ is an arbitrary phase factor. This therefore shows that $|\chi_+\rangle$ and $|\chi_-\rangle$ are related by time-reversal symmetry.

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[35] In our original treatment we have found a nonzero drop due to an error in the derivation of the induced density, i.e. Eq. (14) in Ref. 26 is incorrect.
[36] We treat only the 1D model for simplicity; the generalization of the presented results for several subbands is straightforward.
[37] While in our discussion, we assume identical electrodes in the generalization to a more general case is straightforward and would consist of including a contact potential within the formalism.
[38] This discussion assumes there are only two solutions of the equation $\mu_i=\mu-\tilde{A}|t(\mu_i)|$ which is generally true only if $\tilde{A}$ is smaller than the range of energies where $|t(E)|$ varies significantly. In this case $\mu_{1/2}$ represent the single-particle energies of the right- and left-current carrying states. Only in this respect they correspond to the electro-chemical potential of the right- and left-electrode ($\mu_{R/L}$) present within the Landauer-Büttiker theory.
[39] It is straightforward to show that the small difference in the contribution to the densities $\sim 1/q-1/k$ is not sufficient to remedy the problem of local charge neutrality that appears for $\Delta u \neq 0$.