Variational method with scattering boundary conditions imposed by the Wigner distribution

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A functional form for electrons scattering off localized potentials with boundary conditions imposed through the Wigner distribution function is formulated in a manner appropriate for the study of tunneling in nanoscale junctions. Variation of the functional with respect to the electronic density matrix leads to stationary or critical points respecting open-system boundary conditions. Examples are presented for single-electron and many-(noninteracting) electron scattering and, in both instances, the usual outcome of a one-electron density matrix comprised of scattering wave functions results. The examples highlight how the degrees of freedom associated with imposing scattering boundary conditions can be constrained and removed from a variational determination of the electronic wave functions on a scattering region. The form for the scattering functional is motivated in terms of the maximum entropy principle.

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I. INTRODUCTION

The relationship of scattering to electrical resistance is the hallmark of quantum electronic transport theories.[1] The general framework for variational treatments of time-independent[2] and time-dependent[3] scattering has been known for some time. A many-electron correlated scattering (MECS) treatment for the description of electric current in nanoscale systems has been developed,[4–6] including comparisons to experiment for several molecular tunnel junctions.[7–9] Prediction of electron transport properties across nanoscale tunnel junctions requires application of open-system boundary conditions, and these are typically expressed from a single-particle picture. In addition to the introduction of open-system boundary conditions for nanoscale tunnel junctions and, in particular, for single-molecule tunnel junctions, it is required that an explicit treatment of electron-electron correlations is included in the determination of electric current. Recent work in this area has focused on improving transport theories from a single-electron standpoint[10,11] and directly for many-electron treatments by correcting quasiparticle energies using the GW approximation and related methods[12–15] as well as directly correlated wave-function methods.[4,16]

Theoretical description of electron current across nanoscale junctions can be approached from either a nonequilibrium statistical[17–19] or dynamical theory.[20,21] Statistical approaches concentrate directly on the nonequilbrium density matrix, whereas, if the time evolution for a system driven from equilibrium is followed, attention is usually focused on the nonequilibrium Green's functions (NEGF) description of electron propagation. As emphasized by Jaynes,[19] expectation values and ensemble averages from the two approaches should agree to ensure physical consistency, but the actual means used to build the averages and expectation values from the two approaches are distinct. In this context, the single-particle limit for many-electron correlated scattering[4] will be investigated and shown to be compatible with a wave-function description of electron transport, and formally its relation to a statistical determination of the density matrix for nanoscale junctions is highlighted. In the limit in which electron-electron interactions are ignored, the MECS transport description reduces to noninteracting electrons injected onto a scattering region from electron reservoirs. The MECS method relies on the use of the Wigner phase-space distribution function[22–25] to constrain the system to open boundary conditions. Considering the noninteracting version of the theory enables a direct demonstration that application of scattering boundary conditions through the use of the Wigner distribution function[24] and a variational Ansatz are consistent in the single-particle limit. To perform the analysis, a model previously studied in terms of application of the boundary conditions[26] is revisited. The model is a variant of simple analytical models whereby transmission in one-dimensional channels can be investigated.[27] The version presented here consists of free electrons in left and right electron reservoirs or electrodes described by parabolic energy bands. Noninteracting electrons are incident from the left and right onto a region in which a scattering potential is present, and the form of the potential is chosen to ensure that a voltage difference is found between the left and right electrodes. This is achieved by introduction of the potential step of height V. For the left and right electrode bands, which are filled to a number of states n_F corresponding to the Fermi level, a density matrix for the problem may be immediately written as

$$\rho(q,q') = \frac{1}{l}\left[\sum_{L}^{n_F} \tilde{\psi}_L(q)\tilde{\psi}_L^*(q') + \sum_{R}^{n_F} \tilde{\psi}_R(q)\tilde{\psi}_R^*(q')\right], \quad (1)$$

where $\tilde{\psi}_L, \tilde{\psi}_R$ are electron scattering states incoming from the left and right, respectively, with an incoming normalized flux of l^{-1} per state, q and q' are position variables, and the summation is performed over left L and right R incident electronic states. Spin is not explicitly treated in the analysis, but its inclusion is straightforward. This model is used to demonstrate how a variational method with boundary conditions imposed through the Wigner distribution can be applied to a solution of this many (noninteracting) electron problem but, first, use of the Wigner distribution to impose boundary conditions from a variational treatment of a single-electron scattering problem is presented.

II. VARIATIONAL SINGLE-ELECTRON SCATTERING

In this section, a functional is introduced for the scattering of a single electron off a localized potential in analogy to

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previous works for interacting electrons.[4–6] The functional consists of the sum of the energy expectation value for a single-electron Hamiltonian $\hat{h}$, particle number, and constraint conditions relating the equilibrium or zero-voltage ($V = 0$) and applied-voltage ($V \neq 0$) density matrices as

$$\mathcal{L}[\psi^*,\psi] = \langle\psi|\hat{h}|\psi\rangle - \mu(\langle\psi|\psi\rangle - \eta) + \int_{0^+}^{+\infty} dp\, \lambda_L(p)[f_{\psi\psi^*}(q_L,p) - f_0(q_L,p)] + \int_{-\infty}^{0^-} dp\, \lambda_R(p)[f_{\psi\psi^*}(q_R,p) - f_0(q_R,p)], \quad (2)$$

where $|\psi\rangle$ is in this example a single-electron state, μ is a Lagrangian multiplier associated with normalization, the λ_L and λ_R are Lagrangian multipliers associated with left and right incoming momentum fluxes, and η is the value for the electron wave-function normalization. For the sake of presentation, Eq. (2) is referred to as a quantum transport or electron-scattering (ES) functional. The constraint terms in the functional fix the phase-space distribution functions $f_{\psi\psi^*}$ as voltage is applied to the incoming momentum flux f_0 of left and right electron reservoirs or electrodes at their equilibrium or zero-voltage difference distributions.[28] As a voltage between the left and right electrodes is applied by introducing a potential energy difference across the scattering region $\hat{h} = \hat{h}_0 + \hat{v}$, the *incoming* momentum distributions are constrained to be those from reservoirs locally in equilibrium. As usual, the two reservoirs are allowed to be driven away from equilibrium with respect to one another by application of the voltage difference. The resulting model of a nanoscale tunnel junction is shown schematically in Fig. 1 with the electron reservoirs approximated by free electrons (parabolic energy bands). With this standard description of electrode behavior, the *incoming* momentum distributions for the left and right electrodes do not change with application of voltage.[4,24,26]

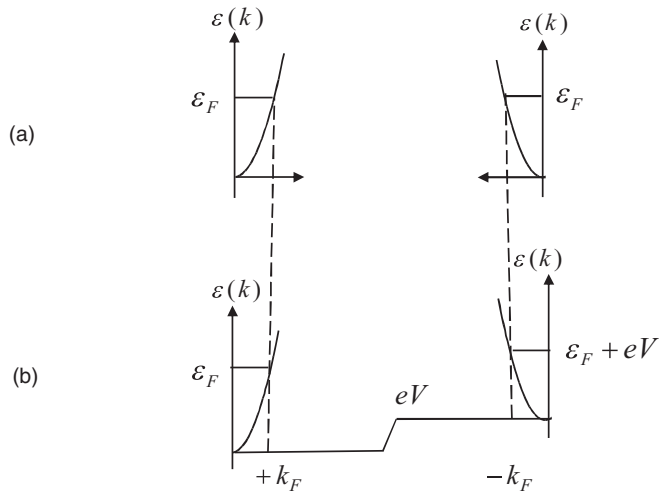

FIG. 1. Electron scattering model. Electron reservoirs described by a single parabolic band emit electrons on a scattering region. The voltage across the scattering region is such that the two-electron reservoirs are driven away from equilibrium with respect to one another. (a) Without application of voltage. (b) With application of voltage.

A. Wigner phase-space distribution function

For the functional equation (2), the phase-space distributions must be specified to allow the incoming flux for momenta to be fixed as needed to describe the open-system boundary conditions. The incoming momenta are constrained by applying the Weyl transformation to the one-electron density matrix generating the Wigner distribution function from the zero-voltage or equilibrium density matrix $\hat{\rho}_0 = |\psi_{V=0}\rangle\langle\psi_{V=0}|$:

$$f_0(q,p) = \int_{-\infty}^{+\infty} ds\, dk\, e^{-ikq-isp}\langle\psi_{V=0}|e^{ik\hat{q}+is\hat{p}}|\psi_{V=0}\rangle, \quad (3)$$

and similarly for the nonequilibrium or $V \neq 0$ density matrix $\hat{\rho} = |\psi\rangle\langle\psi|$ constructed from the one-electron wave functions obtained in the presence of scattering due to the introduction of a potential difference

$$f_{\psi\psi^*}(q,p) = \int_{-\infty}^{+\infty} ds\, dk\, e^{-ikq-isp}\langle\psi|e^{ik\hat{q}+is\hat{p}}|\psi\rangle, \quad (4)$$

a caret is used to denote operators, and specifically is used here to distinguish between position and momentum operators and the Wigner positions and momenta; details of the Weyl transformation as well as it relation to other choices for quantum phase-space distributions are given in Ref. 25.

The Wigner distribution function expresses the density matrix as a phase-space picture consistent with quantum mechanics. Although the choice of a phase-space representation for quantum mechanics is not unique,[25] the Wigner distribution is an appropriate choice to enforce scattering boundary conditions by permitting a description of the electrons emitted from the reservoirs.[24] Momentum expectation values can be written with use of the Wigner distribution as

$$\langle p\rangle = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dp\, dq\ \ p\, f_{\psi\psi^*}(q,p). \quad (5)$$

Equation (5) highlights the use of the Wigner quantum phase-space distribution in analogy to a classical probability distribution function. Unlike a probability distribution, the Wigner function is not everywhere positive[22–25] as a consequence of the momentum-position uncertainty principle. However, in regions where $f_{\psi\psi^*}$ behaves approximately classically, the Wigner distribution function allows us to assign positions and momenta to describe "electrons in the left or right reservoir," "the momentum of an electron emitted from a reservoir," or "a reservoir that is locally in equilibrium." Within this context, the net momentum flow out of a left electrode or electrons incident on a scattering area from the left is approximated as

$$\langle p_L\rangle = \frac{1}{2\pi}\int_{0}^{+\infty} dp\ \ p\ \ f_{\psi\psi^*}(q_L,p), \quad (6)$$

and similarly for the right electrode

$$\langle p_R\rangle = \frac{1}{2\pi}\int_{-\infty}^{0} dp\ \ p\ \ f_{\psi\psi^*}(q_R,p), \quad (7)$$

where q_L and q_R are positions appropriately chosen to describe the equilibrium momentum flow into the scattering region. Clearly, for the above approximations to be appropriate, the Wigner distribution must be used in regions where it well approximates a classical probability distribution. It is

important to note that electrodes are independent of one another as needed to separately maintain local equilibrium in each electrode. In more physical models of tunnel junctions, the density matrix decays rapidly, resulting naturally in a decoupling of the electrodes. To introduce locality into the model considered here, the wave functions will be taken to be nonzero only on the scattering region $[-l/2, +l/2]$. By choosing the electrode Wigner functions to be defined at $q_L = -l/4$ and $q_R = +l/4$ allows decoupling between the left and right "reservoirs" as seen from Eqs. (3) and (4); this choice permits a model description that mimics decoupled electrodes found in quantum transport experiments. To apply the Wigner function to define open boundary conditions for the quantum transport problem, these two conditions must be considered: the application of the boundary conditions are to be applied in regions where the Wigner function may be treated as a semiclassical phase-space distribution function, and the nonlocal character of the Weyl transform requires care when partitioning the transport system into electrode and scattering regions or when applying the Weyl transformation on finite domains to obtain approximations to the Wigner function.[24] Note that these issues are specific to a given description of a model or to numerical calculation, but the one-electron Wigner distribution function is a transformed representation of, and equivalent to, the one-electron reduced density matrix.

B. Variation of the scattering functional

Solutions to the electron-scattering functional are obtained as the stationary points of $\mathcal{L}$ against variation with respect to the density matrix. The resulting variational equation is

$$\begin{aligned}\delta\mathcal{L} = {} & \langle\delta\psi|(\hat{h}-\mu)|\psi\rangle + \langle\psi|(\hat{h}-\mu)|\delta\psi\rangle \\ & + \int_{0^+}^{+\infty} dp\,\lambda_L(p) \int_{-\infty}^{+\infty} ds\,dk\,e^{-ikq_L - isp} \\ & \times(\langle\delta\psi|e^{ik\hat{q}+is\hat{p}}|\psi\rangle + \langle\psi|e^{ik\hat{q}+is\hat{p}}|\delta\psi\rangle) \\ & + \int_{-\infty}^{0^-} dp\,\lambda_R(p) \int_{-\infty}^{+\infty} ds\,dk\,e^{-ikq_R - isp} \\ & \times(\langle\delta\psi|e^{ik\hat{q}+is\hat{p}}|\psi\rangle + \langle\psi|e^{ik\hat{q}+is\hat{p}}|\delta\psi\rangle) = 0. \quad (8)\end{aligned}$$

A scattering region of length l defined between $[-l/2, +l/2]$ is chosen and the Wigner function constraints are applied at $q_L = -l/4$ and $q_R = +l/4$ or in the middle of the "leads" to ensure decoupling of the electrodes. The variation can be written as

$$\begin{aligned}\delta\mathcal{L} = {} & \int_{-l/2}^{+l/2} dq\,[\psi^*(q)(\hat{h}-\mu)\delta\psi(q) + \delta\psi^*(q)(\hat{h}-\mu)\psi(q)] \\ & + \int_{0^+}^{+\infty} dp\,\lambda_L(p) \int_{-l/2}^{+l/2} ds\,e^{-ips}[\delta\psi^*(q_L - s/2) \\ & \times\psi(q_L + s/2) + \psi^*(q_L - s/2)\delta\psi(q_L + s/2)] \\ & + \int_{-\infty}^{0^-} dp\,\lambda_R(p) \int_{-l/2}^{+l/2} ds\,e^{-ips}[\delta\psi^*(q_R - s/2) \\ & \times\psi(q_L + s/2) + \psi^*(q_R - s/2)\delta\psi(q_R + s/2)] = 0, \quad (9)\end{aligned}$$

where $\delta\rho(q,q') = \psi(q)\delta\psi^*(q') + \delta\psi(q)\psi^*(q')$. A single-particle Hamiltonian operator

$$\hat{h} = -\tfrac{1}{2}\partial_q^2 + V(q) \quad (10)$$

is introduced with a potential $V(q)$ assumed constant outside of an interval (a,b) on $[-l/2, +l/2]$ such that the single-electron wave function satisfies

$$\begin{aligned}\psi(q) &\xrightarrow{q\to q_L} Ae^{ikq} + Be^{-ikq}, \\ \psi(q) &\xrightarrow{q\to q_R} Ce^{ik'q} + De^{-ik'q}.\end{aligned} \quad (11)$$

The scattering region defined on $[-l/2,l/2]$ is open, variations at the boundaries do not vanish, and, therefore, the turnover rule is not satisfied, leading to

$$\begin{aligned}& -\frac{1}{2}\int_{-l/2}^{+l/2} dq\,\psi^*(q)\partial_q^2\delta\psi(q) \\ & = -\frac{1}{2}[\partial_q - \partial_{q'}]\psi^*(q')\delta\psi(q)|_{q=q'=-l/2}^{q=q'=+l/2} \\ & \quad - \frac{1}{2}\int_{-l/2}^{+l/2} dq\big[\partial_q^2\psi^*(q)\big]\delta\psi(q) \\ & \equiv -i\,j[\psi^*,\delta\psi]|_{-l/2}^{+l/2} - \frac{1}{2}\int_{-l/2}^{+l/2} dq\big[\partial_q^2\psi^*(q)\big]\delta\psi(q).\end{aligned} \quad (12)$$

The variation of $\mathcal{L}$ becomes

$$\begin{aligned}\delta\mathcal{L} = {} & \int_{-l/2}^{+l/2} dq\left[\delta\psi^*(q)\left(-\frac{1}{2}\overrightarrow{\partial}_q^2 + V(q) - \mu\right)\psi(q) + \psi^*(q)\left(-\frac{1}{2}\overleftarrow{\partial}_q^2 + V(q) - \mu\right)\delta\psi(q)\right] - i\,j[\psi^*,\delta\psi]|_{-l/2}^{+l/2} \\ & + \int_{0^+}^{+\infty} dp\,\lambda_L(p) \int_{-l/2}^{+l/2} ds\,e^{-ips}[\delta\psi^*(q_L - s/2)\psi(q_L + s/2) + \psi^*(q_L - s/2)\delta\psi(q_L + s/2)] \\ & + \int_{-\infty}^{0^-} dp\,\lambda_R(p) \int_{-l/2}^{+l/2} ds\,e^{-ips}[\delta\psi^*(q_R - s/2)\psi(q_R + s/2) + \psi^*(q_R - s/2)\delta\psi(q_R + s/2)] = 0, \quad (13)\end{aligned}$$

where the arrows over the kinetic energy operators indicate the direction in which they operate. A specific form for the potential term is chosen as a step potential, consistent with the requirement of potential energy difference between the left and right electrodes:

$$\hat{h} = -\tfrac{1}{2}\partial_q^2 + V\,\theta(q), \quad (14)$$

with $\theta(q)$ the Heaviside step function and V is the potential step height. This choice for the electron Hamiltonian suffices to demonstrate the use of the Wigner distribution to apply boundary conditions for variational scattering problems; the procedure can be generalized for arbitrary scattering potentials leading to wave functions satisfying Eq. (11). An Ansatz for the wave function is made consistent with the asymptotic form [Eq. (11)] and potential energy choice [Eq. (14)] as

$$\psi(q) = \begin{cases} Ae^{ikq} + Be^{-ikq}, & q < 0 \\ Ce^{ik'q} + De^{-ik'q}, & q > 0. \end{cases} \tag{15}$$

It is clear that the Ansatz may also be written in terms of real expansion functions and appropriately redefined complex coefficients. As usual, the trial wave function is required to be continuous

$$A + B = C + D. \tag{16}$$

The zero-voltage solution for the model as given is for a plane wave incident from the left. The Wigner distribution for the zero-voltage solution[29] is

$$f_0(q,p) = \frac{2\pi}{l}\delta(p-k). \tag{17}$$

For the wave-function Ansatz, the Wigner distribution function is evaluated at $q_L = -l/4$ and $q_R = +l/4$ to yield[29]

$$\begin{aligned} f_{\psi\psi^*}(q_L,p) &= 2\pi|A|^2\delta(p-k) + 2\pi|B|^2\delta(p+k) \\ &\quad + 2\pi(A^*B + AB^*)\cos(2kq)\delta(p), \\ f_{\psi\psi^*}(q_R,p) &= 2\pi|D|^2\delta(p+k') + 2\pi|C|^2\delta(p-k') \\ &\quad + 2\pi(C^*D + CD^*)\cos(2k'q)\delta(p). \end{aligned} \tag{18}$$

It is reiterated that that the wave functions are taken to be nonzero only on the scattering region and the Wigner distributions are determined at the center of the "leads" resulting in the form of $\delta\mathcal{L}$ given in Eq. (13), with decoupling of the density matrix at q_L and q_R achieved as needed for independent electrodes. The rapid decay of the density matrix in metals ensures the decoupling[26,30] found for typical electrode configurations used in quantum transport measurements.

The variation of $\mathcal{L}$ for the choice of $V(q)$ becomes

$$\begin{aligned} \delta\mathcal{L} = &\int_{-l/2}^{0} dq \left[\delta\psi^*(q)\left(-\frac{1}{2}\overrightarrow{\partial}_q^2 - \mu\right)\psi(q) + \psi^*(q)\left(-\frac{1}{2}\overleftarrow{\partial}_q^2 - \mu\right)\delta\psi(q)\right] \\ &+ \int_{0}^{+l/2} dq \left[\delta\psi^*(q)\left(-\frac{1}{2}\overrightarrow{\partial}_q^2 + V - \mu\right)\psi(q) + \psi^*(q)\left(-\frac{1}{2}\overleftarrow{\partial}_q^2 + V - \mu\right)\delta\psi(q)\right] - i\,j[\psi^*,\delta\psi]|_{-l/2}^{+l/2} \\ &+ \int_{0^+}^{+\infty} dp\,\lambda_L(p)\int_{-l/2}^{+l/2} ds\, e^{-ips}[\delta\psi^*(q_L - s/2)\psi(q_L + s/2) + \psi^*(q_L - s/2)\delta\psi(q_L + s/2)] \\ &+ \int_{-\infty}^{0^-} dp\,\lambda_R(p)\int_{-l/2}^{+l/2} ds\, e^{-ips}[\delta\psi^*(q_R - s/2)\psi(q_L + s/2) + \psi^*(q_R - s/2)\delta\psi(q_R + s/2)] = 0, \end{aligned} \tag{19}$$

which, when substituting the wave-function Ansatz (15) into Eq. (19) results in

$$\begin{aligned} \delta\mathcal{L} = &\left(\tfrac{1}{2}k^2 - \mu\right)(A^*\delta A + A\delta A^* + B^*\delta B + B\delta B^*)l/2 + \left(\tfrac{1}{2}k'^2 + V - \mu\right)(C^*\delta C + C\delta C^* + D^*\delta D + D\delta D^*)l/2 \\ &-i(A^*\delta A - B^*\delta B)k + i(C^*\delta C - D^*\delta D)k' + 2\pi\lambda_L(k)(A^*\delta A + A\delta A^*) + 2\pi\lambda_R(k')(D^*\delta D + D\delta D^*) = 0. \end{aligned} \tag{20}$$

The constraint equations relate the zero- and applied-voltage Wigner functions as follows:

$$\begin{aligned} f_{\psi\psi^*}(q_L, p > 0) &= f_0(q_L, p > 0) \\ &= \frac{2\pi}{l}\delta(p-k) \end{aligned} \tag{21}$$

and

$$\begin{aligned} f_{\psi\psi^*}(q_R, p < 0) &= f_0(q_R, p < 0) \\ &= 0. \end{aligned} \tag{22}$$

The constraint equations for the the incoming momentum distributions (21) and (22) require

$$|A|^2 = \frac{1}{l}, \quad p = k, \quad |D|^2 = 0. \tag{23}$$

Considering only variations satisfying the constraint conditions implies that $A^*\delta A + A\delta A^* = D^*\delta D + D\delta D^* = 0$ such that only norm-preserving variations are allowed for these terms. In addition to the momentum constraints, current conservation imposed between the boundaries of the scattering region results in

$$\begin{aligned} j[\psi^*,\delta\psi]|_{-l/2}^{+l/2} &= 0, \\ (A^*\delta A - B^*\delta B)k - C^*\delta C k' &= 0. \end{aligned} \tag{24}$$

The variation of $\mathcal{L}$ becomes

$$\begin{aligned} \left(-\tfrac{1}{2}\partial_q^2 - \mu\right)\psi(q) = 0, \quad q < 0 \\ \left(-\tfrac{1}{2}\partial_q^2 + V - \mu\right)\psi(q) = 0, \quad q > 0 \end{aligned} \tag{25}$$

or

$$\begin{aligned} \tfrac{1}{2}k^2 - \mu &= 0, \\ \tfrac{1}{2}k'^2 + V - \mu &= 0. \end{aligned} \tag{26}$$

It follows that

$$\mu = \tfrac{1}{2}k^2 = \tfrac{1}{2}k'^2 + V. \tag{27}$$

Current continuity and the requirement that the single-particle trial function is continuous leads to

$$\frac{B}{A} = \frac{k-k'}{k+k'} \equiv r_L(k,k'), \quad \frac{C}{A} = \frac{2k}{k+k'} \equiv t_L(k,k'), \tag{28}$$

where r_L and t_L denote the reflected and transmitted coefficients in a scattering wave function incident from the left:

$$\tilde{\psi}_L(q) = \begin{cases} e^{ikq} + r_L(k,k')e^{-ikq}, & q < 0 \\ t_L(k,k')e^{ik'q}, & q > 0 \end{cases} \tag{29}$$

and $\psi(q) = \frac{1}{\sqrt{l}}\tilde{\psi}_L(q)$. Similarly, if the Wigner boundary conditions are chosen such that the incoming momentum is nonzero on the right with no incoming component from the left, the scattering solution takes the standard form for a right incident wave function:

$$\tilde{\psi}_R(q) = \begin{cases} e^{-ik'q} + r_R(k',k)e^{ik'q}, & q > 0 \\ t_R(k',k)e^{-ikq}, & q < 0 \end{cases} \tag{30}$$

with

$$r_R(k',k) = \frac{k'-k}{k+k'}, \quad t_R(k',k) = \frac{2k'}{k+k'}, \tag{31}$$

and $\psi(q) = \frac{1}{\sqrt{l}}\tilde{\psi}_R(q)$.

The preceding calculation demonstrates that a constrained variation of the transport functional equation (2) is consistent with standard textbook descriptions for electron scattering in one dimension (see, e.g., Ref. 31). Use of the Wigner function to impose boundary conditions removes the need for finding a stationary solution for the energy, and then subsequently choosing boundary conditions for the general solution. In terms of mathematical complexity, it may be argued that the procedure as described is no more complicated (or perhaps less so) than applying Green's function methods to the solution of scattering off a potential step in one dimension.[32,33] However, the usefulness of the approach is that it opens the possibility to use the one-electron reduced density matrix to define scattering boundary conditions (as usually formulated within a single-particle picture) to a many-electron wave function, and the many (noninteracting) electron case is examined next.

III. VARIATIONAL MANY- (NONINTERACTING) ELECTRON SCATTERING

The many-electron scattering (MES) model considered is defined for a one-dimensional open system on $[-l/2, +l/2]$ and, at zero voltage, consists of n_F electrons incident from the left and n_F electrons incident from the right, along with any zero-mode terms. In the absence of the voltage, the system consists of free electrons with momenta $k_n = \frac{2\pi}{l}n$ with $n = 0,1,2,3,\ldots$ with positive k states incident from the left, and negative k states incident from the right.[34] The lowest left and right energy states are filled to the Fermi level as depicted in Fig. 1(a) and, in the absence of a voltage difference between electron reservoirs, the current is given by

$$I[V=0] = -\frac{1}{l}\left(\sum_{n\in L}^{n_F} k_n - \sum_{n'\in R}^{n_F} k_{n'}\right) = 0. \tag{32}$$

The free electrons are described by plane waves. In this representation, the density matrix is diagonal, allowing it to be constructed from the first n_F left and right states and the k_0 state (that does not contribute to the current) as

$$\rho_0(q,q') = \frac{1}{l}\Bigg[1 + \sum_{n\in L}^{n_F}\exp[ik_n(q-q')] + \sum_{n'\in R}^{n_F}\exp[-ik_{n'}(q-q')]\Bigg]. \tag{33}$$

Introducing the Weyl transformation term by term, the resulting Wigner distribution function is readily found to be

$$f_0(q,p) = \frac{2\pi}{l}\left[\delta(p) + \sum_{n\in L}^{n_F}\delta(p-k_n) + \sum_{n'\in R}^{n_F}\delta(p+k_{n'})\right], \tag{34}$$

with $\delta(p)$ the Dirac delta function.[29] The many-electron Hamiltonian for the model is

$$\hat{H} = \hat{h}_0 + \sum_{n\in L}^{n_F}\hat{h}_n + \sum_{n'\in R}^{n_F}\hat{h}_{n'} \tag{35}$$

with

$$\hat{h}_n = -\tfrac{1}{2}\partial_{q_n}^2 + V(q_n), \tag{36}$$

and the potential function for each of the electrons taken to be a step-function $V\,\theta(q)$ potential. The wave function for this noninteracting electron system is written as a Slater determinant

$$\Psi = \mathcal{N}\mathcal{A}\,\psi_{k_0}\prod_{n,n'=1}^{n_F}\psi_{L,n}\psi_{R,n'} \equiv \det(\psi_{k_0};\psi_{L,n};\psi_{R,n'}), \tag{37}$$

with $\mathcal{N}$ the normalization and $\mathcal{A}$ denotes the antisymmetrization operator for the electrons. The many-electron version of the scattering functional $\mathcal{L}$ is written[4,5] as

$$\mathcal{L}[\Psi^*,\Psi] = \langle\Psi|\hat{H}|\Psi\rangle - \mu(\langle\Psi|\Psi\rangle - \eta) + \int_{0^+}^{+\infty} dp\,\lambda_L(p)[f_{\Psi\Psi^*}(q_L,p) - f_0(q_L,p)] + \int_{-\infty}^{0^-} dp\,\lambda_R(p)[f_{\Psi\Psi^*}(q_R,p) - f_0(q_R,p)] \tag{38}$$

with the single-electron Wigner function now calculated from the reduced one-electron density matrix obtained from the many-electron wave function Ψ:

$$\rho(q,q') = \int\left[\prod_{n=2}^{2n_F+1} dq_n\right]\Psi(q,q_2,q_3,\ldots)\Psi^*(q',q_2,q_3,\ldots). \tag{39}$$

A. Determining wave-function boundary conditions

To highlight features of the problem absent from the single-electron example, but arising in the many-electron case, the following Ansatz for the single-electron wave functions is made:

$$\begin{aligned} \psi_{L,n}(q) &= A_{L,n}\tilde{\psi}_{L,n}(q) + D_{L,n}\tilde{\psi}_{R,n}(q), \\ \psi_{R,n}(q) &= A_{R,n}\tilde{\psi}_{R,n}(q) + D_{R,n}\tilde{\psi}_{L,n}(q), \end{aligned} \tag{40}$$

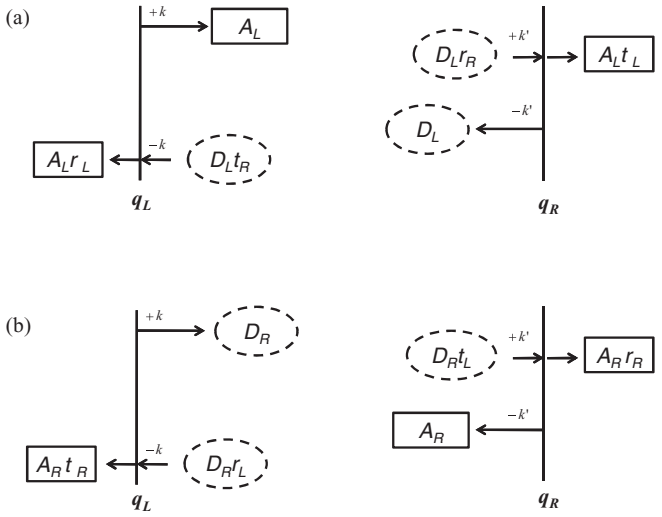

FIG. 2. Wave-function amplitudes for scattering with a degenerate energy pair. (a) Boxes are used to denote amplitudes for a scattering wave function incident from the left, whereas the dashed ovals are used to denote the amplitudes for a scattering wave function incident from the right. (b) Boxes are used to denote amplitudes for a scattering wave function incident from the right, whereas the dashed ovals are used to denote the amplitudes for a scattering wave function incident from the left.

where the $\tilde{\psi}_{L,n}$ and $\tilde{\psi}_{R,n}$ are left and right incident scattering states, respectively,

$$\tilde{\psi}_{L,n}(q) = \begin{cases} e^{ik_n q} + r_L(k_n,k_{n'})e^{-ik_n q}, & q < 0 \\ t_L(k_n,k_{n'})e^{ik_{n'} q}, & q > 0 \end{cases} \tag{41}$$

$$\tilde{\psi}_{R,n}(q) = \begin{cases} e^{-ik_{n'} q} + r_R(k_{n'},k_n)e^{ik_{n'} q}, & q > 0 \\ t_R(k_{n'},k_n)e^{-ik_n q}, & q < 0. \end{cases} \tag{42}$$

In this notation, left and right scattering states $\tilde{\psi}_{L,n}$ and $\tilde{\psi}_{R,n}$ are degenerate in energy and, in terms of momentum, the index n labels the value of the momentum for $q < 0$ for *both* left and right scattering states. The wave-function amplitudes r_L, t_L, r_R, and t_R are defined as in Eqs. (28) and (31). The momentum indices for electrons incident from the left satisfy $1 \leqslant n \leqslant n_F$ and, for right incident electrons, the incident momenta are labeled $1 \leqslant n' \leqslant n_F$. However, with the notation chosen, the energy for a either a left or right incident state is $\epsilon_n = \frac{1}{2}k_n^2$. The relationship between the wave-function amplitudes and momenta for this choice of single-electron wave functions is displayed in Fig. 2. With the Ansatz equation (40), no left or right asymmetry is introduced in the sense that the single-electron trial functions are linear combinations of left and right scattering states. Using this form for the trial functions allows for a demonstration of how open-system boundary conditions can be applied in the many-particle case by removing the balance between left and right states as voltage is applied. The scattering wave functions are eigenfunctions of the single-particle Hamiltonian and the task reduces to finding a set of coefficients in Eq. (40) satisfying scattering boundary conditions.

As voltage is applied, the incoming momentum distributions are fixed, but outgoing momenta are not to be constrained. The notation for the scattering wave functions is such that an incident electron from the left with momentum k_n scatters into a lower momentum state $k_{n'}$, whereas an electron incident from the right with momentum $k_{n'}$ will scatter into a higher momentum state k_n where the two momenta are related by $k_n = \sqrt{k_n'^2 + 2V}$. Right incident states near the bottom of the parabolic energy band will be shifted by the voltage, such that

$$\frac{1}{2}\left(n_V \frac{2\pi}{l}\right)^2 = V, \quad n_V = \sqrt{\frac{V}{2}}\frac{l}{\pi}. \tag{43}$$

Right incident states near the Fermi energy will experience a shift described by

$$\frac{1}{2}\left(n_{\max}\frac{2\pi}{l}\right)^2 = \frac{1}{2}\left(n_F\frac{2\pi}{l}\right)^2 + V, \qquad n_{\max} = \sqrt{n_F^2 + n_V^2}. \tag{44}$$

The lowest left incident states states near the bottom of the parabolic band $n < n_V$ are nonpropagating states. Left incident states near the Fermi level become shifted down in momentum such that the maximum outgoing momentum index becomes $\sqrt{n_F^2 - n_V^2}$. Thus, two cases arise in the many-electron version of the transport model. If a left or right incident electron scatters into a momentum state such that $|k_n|$ is unoccupied for the right or left incident states, respectively, there is no coupling between left and right scattering states and the analysis reverts to a procedure as presented in the preceding section. If the incident states scatter into a state such that their wave functions couple through the constraint conditions, this implies the left and right states are degenerate in energy, and this case is examined next.

The many-electron scattering functional is written in terms of the single-electron Hamiltonians $\hat{h}$ and wave functions $\psi_{L,n}, \psi_{R,n}$, and for states degenerate in energy, the contribution to the functional is[29]

$$\begin{aligned} \mathcal{L}_n[\Psi^*,\Psi] = {} & \langle\psi_{L,n}|\hat{h}_n|\psi_{L,n}\rangle + \langle\psi_{R,n}|\hat{h}_n|\psi_{R,n}\rangle - \mu_{L,n}[\langle\psi_{L,n}|\psi_{L,n}\rangle - \eta_{L,n}] - \mu_{R,n}[\langle\psi_{R,n}|\psi_{R,n}\rangle - \eta_{R,n}] \\ & + 2\pi\int_{0^+}^{+\infty} dp\,\lambda_L(p)\left[\left(|A_{L,n}|^2 + |D_{R,n}|^2 - \frac{1}{l}\right)\delta(p-k_n)\right] \\ & + 2\pi\int_{-\infty}^{0^-} dp\,\lambda_R(p)\left[\left(|A_{R,n}|^2 + |D_{L,n}|^2 - \frac{1}{l}\right)\delta(p+k_{n'})\right], \end{aligned} \tag{45}$$

with $\mu = \sum(\mu_{L,n} + \mu_{R,n})$ and $\eta = \sum(\eta_{L,n} + \eta_{R,n})$. The constraints on the momentum distributions in this case yield

$$\begin{aligned} |A_{L,n}|^2 + |D_{R,n}|^2 &= \frac{1}{l}, \\ |A_{R,n}|^2 + |D_{L,n}|^2 &= \frac{1}{l}. \end{aligned} \tag{46}$$

Scattering states $\tilde{\psi}$ are orthogonal[35] and the single-particle solutions [Eq. (40)] are to be constructed as orthogonal. Requiring $\langle \psi_{L,n} | \psi_{R,n} \rangle = 0$ for degenerate energy states in Eq. (40) imposes a relationship for the trial wave-function amplitudes

$$\begin{aligned} A^*_{L,n} D_{R,n} + A_{R,n} D^*_{L,n} &= 0, \\ A_{L,n} D^*_{R,n} + A^*_{R,n} D_{L,n} &= 0. \end{aligned} \tag{47}$$

These relations are written, using the norms and arguments of the complex amplitudes, as

$$\begin{aligned} &|A_{L,n}||D_{R,n}| \exp\left[-i(\theta_{A_{L,n}} - \theta_{D_{R,n}})\right] \\ &\quad + |A_{R,n}||D_{L,n}| \exp\left[i(\theta_{A_{R,n}} - \theta_{D_{L,n}})\right] = 0, \\ &|A_{L,n}||D_{R,n}| \exp\left[i(\theta_{A_{L,n}} - \theta_{D_{R,n}})\right] \\ &\quad + |A_{R,n}||D_{L,n}| \exp\left[-i\left(\theta_{A_{R,n}} - \theta_{D_{L,n}}\right)\right] = 0, \end{aligned} \tag{48}$$

and together as

$$\begin{aligned} &|A_{L,n}||D_{R,n}| \cos\left(\theta_{A_{L,n}} - \theta_{D_{R,n}}\right) \\ &\quad + |A_{R,n}||D_{L,n}| \cos\left(\theta_{A_{R,n}} - \theta_{D_{R,n}}\right) = 0. \end{aligned} \tag{49}$$

Consistent with the assumption of independent electrodes, only solutions not introducing phase correlations between the electron reservoirs (see Fig. 2) need be considered,[36] yielding that $|A_{L,n}| = 0$ or $|D_{R,n}| = 0$, and $|A_{R,n}| = 0$ or $|D_{L,n}| = 0$. Selecting, for example, $|D_{R,n}| = 0$ implies $A_{L,n} = \frac{1}{\sqrt{l}} \exp(i\theta_{A_{L,n}})$ from the flux condition (46). Consequently, from $|\psi_{R,n}\rangle \neq 0$ then $A_{R,n} \neq 0$ requiring $D_{L,n} = 0$. Then, $A_{R,n} = \frac{1}{\sqrt{l}} \exp(i\theta_{A_{R,n}})$ from the flux condition.

The one-electron density matrix can now be written in terms of the wave functions [Eq. (40)] as

$$\rho(q,q') = \sum_n \rho_n(q,q'). \tag{50}$$

For nondegenerate states, the contribution to the density matrix is

$$\begin{aligned} \rho_n(q,q') &= |A_{L,n}|^2 \tilde{\psi}_{L,n}(q) \tilde{\psi}^*_{L,n}(q') \\ &= \frac{1}{l} \tilde{\psi}_{L,n}(q) \tilde{\psi}^*_{L,n}(q') \end{aligned} \tag{51}$$

or

$$\begin{aligned} \rho_n(q,q') &= |A_{R,n}|^2 \tilde{\psi}_{R,n}(q) \tilde{\psi}^*_{R,n}(q') \\ &= \frac{1}{l} \tilde{\psi}_{R,n}(q) \tilde{\psi}^*_{R,n}(q'). \end{aligned} \tag{52}$$

For degenerate states, the coupling introduced by the momentum distribution constraints between the left and right states and the orthonormality of $\psi_{L,n}$ and $\psi_{R,n}$ lead to

$$\begin{aligned} \rho_n(q,q') &= (|A_{L,n}|^2 + |D_{R,n}|^2) \tilde{\psi}_{L,n}(q) \tilde{\psi}^*_{L,n}(q') + (|A_{R,n}|^2 \\ &\quad + |D_{L,n}|^2) \tilde{\psi}_{R,n}(q) \tilde{\psi}^*_{R,n}(q') \\ &= \frac{1}{l} [\tilde{\psi}_{L,n}(q) \tilde{\psi}^*_{L,n}(q') + \tilde{\psi}_{R,n}(q) \tilde{\psi}^*_{R,n}(q')], \end{aligned} \tag{53}$$

resulting in

$$\rho(q,q') = \frac{1}{l} [\sum_L^{n_F} \tilde{\psi}_L(q) \tilde{\psi}^*_L(q') + \sum_R^{n_F} \tilde{\psi}_R(q) \tilde{\psi}^*_R(q')] \tag{54}$$

ignoring zero-mode terms. The density matrix determined from the energy functional with boundary conditions imposed through the Wigner function is equivalent to solving the Schrödinger equation for single-electron scattering states with fixed incoming flux l^{-1} and occupying the first n_F of these right and left incoming states. As the one-electron reduced density matrices for the two descriptions are equivalent, all one-electron properties calculated will be equivalent. In particular, the current density

$$j(q) = \frac{1}{2i} [\partial_q - \partial_{q'}] \rho(q,q')|_{q=q'} \tag{55}$$

will be identical for any solution to Eq. (38), satisfying the form for single-particle wave functions [Eq. (40)], the flux condition [Eq. (46)], and the orthogonality condition [Eq. (47)] for degenerate energy states. A solution for electrons with left and right scattering wave functions resulting from the choice of $A_{L,n} = A_{R,n} = \frac{1}{\sqrt{l}}$ and $D_{L,n} = D_{R,n} = 0$ is equivalent to the set of solutions obeying the stationary condition for the MES transport functional [Eq. (38)]. With the single-electron wave-function Ansatz as chosen, variation of $\mathcal{L}$ is not needed, although the resulting solution is stationary against variations with respect to the density matrix. The scattering boundary conditions as expressed through the Wigner distribution are sufficient to select the appropriate solutions and provide the standard description of electrons emitted from reservoirs.

B. A more general wave-function Ansatz

Solution of the MES transport functional [Eq. (38)] with an Ansatz for the single-particle wave functions with variational degrees of freedom that do not directly enter the constraint equations is now performed. The following form for the trial single-particle functions is made analogously to Sec. II:

$$\psi_{L,n}(q) = \begin{cases} A_{L,n} e^{ik_n q} + B_{L,n} e^{-ik_n q}, & q < 0 \\ C_{L,n} e^{ik_{n'} q} + D_{L,n} e^{-ik_{n'} q}, & q > 0 \end{cases} \tag{56}$$

$$\psi_{R,n}(q) = \begin{cases} A_{R,n} e^{-ik_{n'} q} + B_{R,n} e^{ik_{n'} q}, & q > 0 \\ C_{R,n} e^{-ik_n q} + D_{R,n} e^{ik_n q}, & q < 0 \end{cases} \tag{57}$$

and the trial wave functions are again required to be continuous. To explicitly solve for the trial functions, stationarity of the scattering functional is required. For nondegenerate states, the many-electron variation leads to a sum of independent particle variations and these may be solved by using the procedure given in Sec. II. However, as in the preceding section, where the constraint conditions on the momentum distributions introduce coupling between left and right states degenerate in energy, a slightly modified approach is required for degenerate states. The many-electron variation leads to

$$\begin{aligned}\delta\mathcal{L}_n = \int_{-l/2}^{+l/2} dq \;& [\delta\psi^*_{L,n}(q)(\hat{h}_n-\mu_{L,n})\psi_{L,n}(q)+\delta\psi_{L,n}(q)\,(\hat{h}_n-\mu_{L,n})\psi^*_{L,n}(q)\\ &+\delta\psi^*_{R,n}(q)(\hat{h}_n-\mu_{R,n})\psi_{R,n}(q)+\delta\psi_{R,n}(q)(\hat{h}_n-\mu_{R,n})\psi^*_{R,n}(q)]\\ &-i\{j[\psi^*_{L,n},\delta\psi_{L,n}]+\;j[\psi^*_{R,n},\delta\psi_{R,n}]\}|^{+l/2}_{-l/2}\\ +\int_{0^+}^{+\infty} dp\,\lambda_L(p)\int_{-l/2}^{+l/2} ds\,e^{-ips} \;& [\delta\psi^*_{L,n}(q_L-s/2)\psi_{L,n}(q_L+s/2)+\;\psi^*_{L,n}(q_L-s/2)\delta\psi_{L,n}(q_L+s/2)\\ &+\delta\psi^*_{R,n}(q_L-s/2)\psi_{R,n}(q_L+s/2)+\psi^*_{R,n}(q_L-s/2)\delta\psi_{R,n}(q_L+s/2)]\\ +\int_{-\infty}^{0^-} dp\,\lambda_R(p)\int_{-l/2}^{+l/2} ds\,e^{-ips} \;& [\delta\psi^*_{L,n}(q_R-s/2)\psi_{L,n}(q_R+s/2)+\psi^*_{L,n}(q_R-s/2)\delta\psi_{L,n}(q_R+s/2)\\ &+\delta\psi^*_{R,n}(q_R-s/2)\psi_{R,n}(q_R+s/2)+\psi^*_{R,n}(q_R-s/2)\delta\psi_{R,n}(q_R+s/2)]=0 \end{aligned} \tag{58}$$

for left and right states degenerate in energy. A single-particle Hamiltonian of the form $\hat{h}_n = -\frac{1}{2}\partial^2_{q_n} + V\theta(q_n)$ is again selected and the variation $\delta\mathcal{L}_n$ becomes

$$\begin{aligned}\delta\mathcal{L}_n = &\left(\tfrac{1}{2}k_n^2-\mu_{L,n}\right)(A^*_{L,n}\delta A_{L,n}+A_{L,n}\delta A^*_{L,n}+B^*_{L,n}\delta B_{L,n}+B_{L,n}\delta B^*_{L,n})l/2\\ &+\left(\tfrac{1}{2}k_{n'}{}^2+V-\mu_{L,n}\right)(C^*_{L,n}\delta C_{L,n}+C_{L,n}\delta C^*_{L,n}+D^*_{L,n}\delta D_{L,n}+D_{L,n}\delta D^*_{L,n})l/2\\ &+\left(\tfrac{1}{2}k_{n'}{}^2+V-\mu_{R,n}\right)(A^*_{R,n}\delta A_{R,n}+A_{R,n}\delta A^*_{R,n}+B^*_{R,n}\delta B_{R,n}+B_{R,n}\delta B^*_{R,n})l/2\\ &+\left(\tfrac{1}{2}k_n^2-\mu_{R,n}\right)(C^*_{R,n}\delta C_{R,n}+C_{R,n}\delta C^*_{R,n}+D^*_{R,n}\delta D_{R,n}+D_{R,n}\delta D^*_{R,n})l/2\\ &-i(A^*_{L,n}\delta A_{L,n}-B^*_{L,n}\delta B_{L,n}-C^*_{R,n}\delta C_{R,n}+D^*_{R,n}\delta D_{R,n})k_n\\ &-i(A^*_{R,n}\delta A_{R,n}-B^*_{R,n}\delta B_{R,n}-C^*_{L,n}\delta C_{L,n}+D^*_{L,n}\delta D_{L,n})k_{n'}\\ &+2\pi\lambda_L(k_n)(A^*_{L,n}\delta A_{L,n}+A_{L,n}\delta A^*_{L,n}+D^*_{R,n}\delta D_{R,n}+D_{R,n}\delta D^*_{R,n})\\ &+2\pi\lambda_R(k_{n'})(A^*_{R,n}\delta A_{R,n}+A_{R,n}\delta A^*_{R,n}+D^*_{L,n}\delta D_{L,n}+D_{L,n}\delta D^*_{L,n})=0. \end{aligned} \tag{59}$$

The constraint conditions for the momentum distributions yield

$$\begin{aligned}|A_{L,n}|^2+|D_{R,n}|^2=\frac{1}{l},\\ |A_{R,n}|^2+|D_{L,n}|^2=\frac{1}{l},\end{aligned} \tag{60}$$

leading to variations satisfying

$$\begin{aligned}A^*_{L,n}\delta A_{L,n}+A_{L,n}\delta A^*_{L,n}+D^*_{R,n}\delta D_{R,n}+D_{R,n}\delta D^*_{R,n}=0,\\ A^*_{R,n}\delta A_{R,n}+A_{R,n}\delta A^*_{R,n}+D^*_{L,n}\delta D_{L,n}+D_{L,n}\delta D^*_{L,n}=0.\end{aligned} \tag{61}$$

Requiring the single-electron currents entering and leaving the scattering region to cancel requires that

$$\begin{aligned}&(A^*_{L,n}\delta A_{L,n}-B^*_{L,n}\delta B_{L,n})k_n\\ &\quad-(C^*_{L,n}\delta C_{L,n}-D^*_{L,n}\delta D_{L,n})k_{n'}=0,\\ &-(A^*_{R,n}\delta A_{R,n}-B^*_{R,n}\delta B_{R,n})k_{n'}\\ &\quad+(C^*_{R,n}\delta C_{R,n}-D^*_{R,n}\delta D_{R,n})k_n=0.\end{aligned} \tag{62}$$

The variation of $\mathcal{L}$ becomes

$$\begin{aligned}\left(-\tfrac{1}{2}\partial_q^2-\mu_{L,n}\right)\psi_{L,n}(q)=0, \qquad q<0\\ \left(-\tfrac{1}{2}\partial_q^2-\mu_{R,n}\right)\psi_{R,n}(q)=0, \qquad q<0\\ \left(-\tfrac{1}{2}\partial_q^2+V-\mu_{L,n}\right)\psi_{L,n}(q)=0, \qquad q>0\\ \left(-\tfrac{1}{2}\partial_q^2+V-\mu_{R,n}\right)\psi_{R,n}(q)=0, \qquad q>0\end{aligned} \tag{63}$$

or

$$\mu_{L,n}=\mu_{R,n}=\tfrac{1}{2}k^2=\tfrac{1}{2}k'^2+V. \tag{64}$$

Current continuity combined with the requirement that the single-electron wave functions are continuous leads to

$$\begin{aligned}B_{L,n}&=A_{L,n}r_L(k_n,k_{n'})+D_{L,n}t_R(k_{n'},k_n),\\ C_{L,n}&=A_{L,n}t_L(k_n,k_{n'})+D_{L,n}r_R(k_{n'},k_n),\\ B_{R,n}&=A_{R,n}r_R(k_{n'},k_n)+D_{R,n}t_L(k_n,k_{n'}),\\ C_{R,n}&=A_{R,n}t_R(k_{n'},k_n)+D_{R,n}r_L(k_n,k_{n'}),\end{aligned} \tag{65}$$

where the reflection r and transmission amplitudes t for left and right scattering states are for the case of a potential step given in Eqs. (28) and (31). This permits the left and right eigenstates expressed in terms of the scattering wave functions to be written as in Eq. (40). As noted previously, written in this form, the reduced one-electron density matrix is equivalent to a solution built separately from left and right scattering states with normalized incoming flux l^{-1} for each state. Hence, all one-electron properties including electron current are identical between the set of solutions defined by the constraint conditions (60) and the standard solutions for scattering states incident on a potential step with amplitudes given by $A_{L,n}=A_{R,n}=1/\sqrt{l}$ and $D_{L,n}=D_{R,n}=0$.

IV. CONDUCTANCE QUANTIZATION

In the preceding section, it has been shown that variation of the MES functional [Eq. (38)] leads to a density matrix for many noninteracting electrons that lead to a one-electron density matrix equivalent to defining a system of electrons described by scattering wave functions and fixing the incoming flux to prescribed boundary conditions. It has previously been shown that this leads to a prediction of conductance quantization in the linear-response limit.[26] For completeness, the steps leading to a calculation of the conductance quantum within the model are outlined.

As voltage is applied, electrons incident from the left with energies such that $\mu_n/e < V$ will see a potential step up, where e is the electronic charge (in the following all physical quantities are explicit). The number of these states is given approximately as

$$n_V \approx \sqrt{2emV}/\hbar\Delta k, \tag{66}$$

where m is the electron mass, $\hbar$ is Planck's constant h divided by 2π, and $\Delta k = \frac{2\pi}{l}$ is the momentum spacing. For scattering states incoming from the left, the electron transmission is approximated as $T_{L,n} \sim 0$ for incoming energies less than the potential step-up height, and $T_{L,n} = \frac{k'_n}{k_n} t^2_{L,n} \sim 1$ for energies greater than the potential step. In contrast, electrons incident from the right see a step-down potential and we approximate the transmission as $T_{R,n} = \frac{k_n}{k_{n'}} t^2_{R,n} \sim 1$ for all right incident electrons. The electron current within this approximation is

$$\begin{aligned} I &\sim -\frac{e\hbar}{ml}\left[\sum_{n=n_V}^{n_F} k_n - \sum_{n=1}^{n_F} k_n\right] \\ &\sim \frac{e\hbar}{ml}\sum_{n=1}^{n_V} k_n \\ &\sim \frac{e\hbar}{ml}\sum_{n=1}^{n_V} n\Delta k, \end{aligned} \tag{67}$$

with the convention that electron current is opposite the direction of electron flow. For $1 \ll n_V \ll n_F$,

$$I \to \frac{e\hbar}{ml}\Delta k \int_0^{n_V} n\, dn = \frac{e^2}{h} V. \tag{68}$$

The current and voltage yield a conductance $g_0 = I/V = e^2/h$ in agreement with the linear-response result for conductance quantization.

V. RELATION TO MAXIMUM ENTROPY DENSITY MATRIX

The form of the scattering functionals for the one-electron and many-electron cases [Eqs. (2) and (38)] is now motivated in relation to the maximum entropy principle.[17,37] Following von Neumann and Shannon,[37,38] the information entropy of a probability distribution is quantified by

$$S = -\mathrm{Tr}\,\hat{\rho}\ln\hat{\rho}. \tag{69}$$

It is assumed that the energy and particle number can be expressed as

$$\langle E\rangle = \mathrm{Tr}\,\hat{H}\,\hat{\rho}, \quad \langle\eta\rangle = \mathrm{Tr}\,\hat{\rho}, \tag{70}$$

respectively.[39] The scattering region is in contact with two-electron reservoirs or electrodes, and in addition to the energy expectation and normalization, the functionals (2) and (38) introduce terms fixing the incoming momentum distributions to equilibrium ($V = 0$) values characteristic of the electrodes or leads. The Wigner function is a convenient means for approximately describing the incoming momentum flow and can be expressed in the form

$$f(q_{L/R}, p_i) = \mathrm{Tr}\,\hat{F}(q_{L/R}, p_i)\,\hat{\rho}, \tag{71}$$

where the $\hat{F}(q_{L/R}, p_i)$ are the operators expressing the Weyl transform of the density matrix. Hence, it is assumed that the relevant information to describe scattering is the energy on the region, normalization, and the incoming equilibrium momentum distributions for the electrons, the reservoir boundary conditions.[24] Entropy is maximized subject to constraints corresponding to the expectation values

$$\begin{aligned} \max\Bigg[S - \mu\,\mathrm{Tr}\hat{\rho} - \beta\,\mathrm{Tr}\,\hat{H}\,\hat{\rho} - \sum_{p_i>0}\lambda_L(p_i)\mathrm{Tr}\,\hat{F}(q_L,p_i)\,\hat{\rho} \\ - \sum_{p_i<0}\lambda_R(p_i)\mathrm{Tr}\,\hat{F}(q_R,p_i)\,\hat{\rho}\Bigg], \end{aligned} \tag{72}$$

where the Lagrangian multipliers μ, β, and $\lambda_{L/R}(p_i)$ are introduced. Maximizing entropy with respect to variations $\delta\rho$ results in a density matrix of the form

$$\begin{aligned} \hat{\rho} = \exp\Bigg[-\mu - \beta\hat{H} - \sum_{p_i>0}\lambda_L(p_i)\hat{F}(q_L,p_i) \\ - \sum_{p_i<0}\lambda_R(p_i)\hat{F}(q_R,p_i)\Bigg]. \end{aligned} \tag{73}$$

The quantum transport ensemble thus satisfies

$$\begin{aligned} S_{\max} = \mu\,\mathrm{Tr}\,\hat{\rho} + \beta\,\mathrm{Tr}\,\hat{H}\,\hat{\rho} + \sum_{p_i>0}\lambda_L(p_i)\mathrm{Tr}\,\hat{F}(q_L,p_i)\,\hat{\rho} \\ + \sum_{p_i<0}\lambda_R(p_i)\mathrm{Tr}\,\hat{F}(q_R,p_i)\,\hat{\rho}, \end{aligned} \tag{74}$$

and, together with the requirement that the Lagrangian multipliers are chosen to fix the expectation values [Eqs. (70) and (71)], provides the motivation for seeking stationary solutions for functionals of the form of Eqs. (2) and (38), following minor redefinition of the Lagrangian multipliers. The benefit of this approach to quantum transport is that it enables direct application of scattering boundary conditions to a correlated density matrix.[4,6,26] For this case, the many-electron Hamiltonian contains two-electron interactions $\sum_n \hat{h}_n + \sum_{n'<n}\hat{v}_{n'n} \to \hat{H}$. Again, stationary solutions for the functional

$$\begin{aligned} \mathcal{L}[|\Psi_N\rangle\langle\Psi_N|] &= \mathcal{L}[\hat{\rho}_N] \\ &= \mu(\mathrm{Tr}_1\hat{\rho}_1 - \eta) + \beta[\mathrm{Tr}_1\hat{h}\hat{\rho}_1 + \mathrm{Tr}_2\hat{v}\hat{\rho}_2] \\ &\quad + \sum_{p_i>0}\lambda_L(p_i)[\mathrm{Tr}_1\hat{F}(q_L,p_i)\hat{\rho}_1 - f_0(q_L,p_i)] \\ &\quad + \sum_{p_i<0}\lambda_R(p_i)[\mathrm{Tr}_1\hat{F}(q_R,p_i)\hat{\rho}_1 - f_0(q_R,p_i)] \end{aligned} \tag{75}$$

are sought, where $\hat{\rho}_1$ and $\hat{\rho}_2$ are appropriately normalized one- and two-electron reduced density matrices, respectively, obtained from a tracing over $N-1$ and $N-2$ coordinates in a correlated N-body density matrix $|\Psi_N\rangle\langle\Psi_N|$ defined on the scattering region. As a chemical potential is applied to drive the electron reservoirs away from equilibrium with respect to one another, the resulting density matrix describes the scattering in the region coupled to the two reservoirs.

VI. CONCLUSION

The theory examined in this paper provides a demonstration of the use of boundary conditions as constraints to describe electron scattering and represents the single-particle limit to MECS.[4] It should be noted that *any* set of boundary conditions expressible through the Wigner distribution function can be used to constrain the density matrix boundary conditions describing reservoirs in equilibrium at any temperature, *or* quasiequilibrium electron distributions in leads connecting electron reservoirs to the scattering region can equally well be described. In the example of the latter case, leads in equilibrium with an electron reservoir are important to generate atomic-scale models for electron transport.

This work motivates use of the constrained variations to generate correlated transport solutions for molecular electronics[7–9] and related quantum transport problems, in that it demonstrates how a many-electron wave function can be generated satisfying scattering boundary conditions imposed on the one-electron reduced density matrix. In this way, appropriate boundary conditions describing incoming electrons as needed to break time-reversal symmetry[24] are achieved. This study focused on noninteracting electrons in one spatial dimension, whereas previous applications of this approach have been given for three-dimensional systems of correlated electrons. Use of a single-particle model allows for an explicit demonstration that the maximum entropy principle combined with a variational determination of the density matrix subject to scattering boundary conditions is consistent with standard formulations of electron transport. The calculations presented demonstrate how the degrees of freedom associated with imposing scattering boundary conditions can be fixed and removed from a variational determination of the electronic wave functions on a scattering region. The advantage of the method is that it can be readily generalized to the case of correlated electrons[4] using computational many-electron methods.[40–42]

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