II. THEORY

In order to proceed, let us consider the entropy per unit area of the two-dimensional electron gas to be a functional of the electronic occupancies given by\(^\text{10}\).
\[ S[f(k)] = - \int \frac{d^2k}{2\pi^2} (f(k) \ln f(k) + [1 - f(k)] \ln [1 - f(k)]). \]

(1)

The electronic occupancies are written as

\[ f(k) = \begin{cases} f_L(k) & \text{if } k_x < 0 \\ f_R(k) & \text{if } k_x > 0, \end{cases} \]

where \( k = (k_x, k_y) \) and \( f_{LR} \) are the occupation functions to be varied independently in order to maximize Eq. (1) with constraints on the average total energy per unit area and different average numbers of left- and right-moving particles per unit area. In our model, the two-dimensional electron gas is assumed to be embedded between two reservoirs characterized by two different electrochemical potentials. The reservoirs effectively constrain the numbers of left- and right-moving states to be different in the gas, and hence, we add this constraint to our maximization procedure. We represent our knowledge about the system’s constituents and their interactions by the many-electron interacting Hamiltonian together with the Hartree-Fock (i.e., exchange-only) approximation to the many-body wave function. In such a model, at zero or nonzero temperatures, the expectation value of the Hamiltonian is given by

\[ \langle E \rangle = 2 \int \frac{d^2k}{(2\pi)^2} f(k) k^2 \]

\[ - \int \frac{d^2k'}{(2\pi)^2} \int \frac{d^2k}{(2\pi)^2} f(k) f(k') v(k, k'), \]

(2)

where \( v(k, k') = 2\pi/|k - k'| \) is the Fourier transform of the Coulomb interaction in two dimensions. The number of left- and right-moving electrons per unit area can be written as

\[ n_{L(R)} = \frac{1}{(2\pi)^2} \int_{k_x < (>) 0} d^2k f_{L(R)}(k). \]

(3)

In order to maximize the entropy functional with respect to \( f_{LR} \), subject to the above-mentioned constraints, we use the method of Lagrange multipliers and consider the auxiliary functional

\[ \mathcal{L}[f(k)] = S - \beta \langle E \rangle - \mu_L n_L - \mu_R n_R, \]

(4)

together with the extremal condition

\[ \frac{\delta \mathcal{L}}{\delta f_{LR}} = 0. \]

(5)

A straightforward calculation shows that the occupation functions that maximize the entropy functional with constraints in the above-mentioned averages are given by

\[ f_{L(R)}(k) = \frac{1}{1 + \exp[\beta(k^2/2 + \epsilon(k) - \mu_{LR})]}, \]

(6)

where

\[ \epsilon(k) = -\frac{1}{(2\pi)^2} \int_{k_x < 0} d^2k' f_L(k') v(k, k'). \]

(7)

In the nonequilibrium regime, the exchange hole is elongated along the direction of the current. The contours are at \( g = 0.5, 0.75, 0.9, \) and 0.95. (b) Difference between the equilibrium and nonequilibrium holes, \( \Delta g \) (see text). The contours are drawn at 0.1 (dashed), –0.1 (dotted), and 0 (dotted). \( \Delta g \) is oscillating, integrates to zero, and has a marked antisymmetric character. Thus, the current dependence of the local exchange potential and exchange energy is expected to be weak.

\[ \epsilon_x = -\frac{1}{(2\pi)^2} \int_{k_x < 0} d^2k' f_L(k') v(k, k'). \]

(8)

A Hartree-Fock pair distribution function

Let us begin by discussing the current dependence of the Hartree-Fock pair distribution function for spindlike electrons, which is given by

\[ g(r, r') = 1 - \frac{1}{n} \int \frac{d^2k}{(2\pi)^2} \exp[-i \mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')] f(k) \]

(8)

and shown for \( n_L/n_R = 0.5 \) in Fig. 1(a). For \( n_L = n_R \), \( g \) is spherically symmetric, while for \( n_L \neq n_R \) is elongated in the direction of the current. Similar phenomenology has been reported previously by Skudlarski and Vignale for the three-
dimensional electron gas in the presence of a magnetic field,\textsuperscript{12} where the exchange hole is elongated in the direction of the field. In Ref. 12, the elongation arises from the change of occupancies associated with the Zeeman splitting due to the externally applied magnetic field. In the present case, the elongation of the hole can be understood in terms of the change in the electronic occupancies that results from our constrained maximization of the entropy functional. In both cases, the elongation of the hole is the result of the change in the polarizability induced by the change in the occupancies.\textsuperscript{12} As argued in Ref. 12, when correlations are included the isotropy of the Coulomb interaction will bring the shape of the pair-probability distribution back to a more spherical form and, thus, closer to equilibrium.

Note that the difference between the equilibrium and nonequilibrium exchange holes, $\Delta g=g_{eq}-g_{nep}$, shown in Fig. 1(b), has a strong antisymmetric character; i.e., defining $R=r-r'=(X,Y)$, then $\Delta g(X,Y)=-\Delta g(Y,X)$. We shall return to this point later when discussing the weak dependence of the exchange energy on the current density.

### B. Single-particle spectrum

Figure 2 shows the self-consistent single-particle energy spectrum. Figure 2(a) shows the total (kinetic+exchange) spectrum, while in Fig. 2(b), we plotted only its exchange part on the $k_z=0$ line as given by Eq. (7) for $n_L=n_R$ and $n_L/n_R=0.5$.

The combined effect of the constraints and the exchange interaction shifts the spectrum toward higher values of $k_z$. Note also that, when compared to the equilibrium spectrum, the minimum of the nonequilibrium spectrum is less negative. Hence, we expect the total nonequilibrium exchange energy to increase with respect to the equilibrium one. Note that the constraints alter the total kinetic energy of the system, but do not change the kinetic contribution to the single-particle spectrum, since this contribution does not depend on the electronic occupancies. Hence, the changes in the single-particle spectrum are entirely due to the exchange interaction, which raises (lowers) the single-particle energy of electrons with $k_z<0$ ($k_z>0$). The anomalous behavior in the $k_z=0$ plane inherited from the discontinuous character of the maximum entropy momentum distribution can be seen clearly in Fig. 2(a), between $\mu_L$ and $\mu_R$.

The interplay between nonequilibrium occupancies and the single-particle spectrum observed here is just a consequence of the orbital dependence of the Fock operator and the Keldysh-nonequilibrium Green’s function (NEGF) formalism, with an orbital-dependent description of the interactions between the electrons, such as the Hartree-Fock approximation.

We would like to point out that practical implementations of NEGF formalism typically take the electronic structure of the leads to be that of the equilibrium system (see Ref. 13 and references therein),\textsuperscript{16} and hence, the dependence of the single-particle spectrum on the nonequilibrium current (and vice versa) is commonly ignored. The validity of this approximation is geometry dependent: it works in quantum point contact geometries, while it does not in planar electrode geometries at high currents. As a consequence, under the “noninteracting equilibrium lead approximation,” the distribution of incoming electrons would be current independent, while, as this example shows,\textsuperscript{17} the unavoidable presence of interactions in the leads induces a current dependence in the nonequilibrium occupancies through the exchange part of the single-particle spectrum. Unless the geometry is adequately chosen, the distribution of incoming electrons will be that of a nonequilibrium lead such as ours.

In order to capture this subtle effect within the NEGF type of approaches, the coupling self-energy needs to be obtained from the lead’s Green’s function, which includes the necessary current dependence of the Fock operator. This can be achieved within a self-consistent scheme where not only the central region but also the leads’ Green’s functions are calculated self-consistently, as we have discussed in Ref. 13, with the nonlocal Fock operator being used within the whole system (electrodes and the central region).

### C. Total energy

Once the self-consistent single-particle spectrum is calculated, the total exchange energy $E_x$ can be obtained from the second term in the right hand side of Eq. (2). Figure 3 shows the dependence of the $r_x$-invariant quantity $-\epsilon_x/E_{eq}$ on $(1-n_L/n_R)$. For $n_L/n_R=0.25$, the exchange energy deviates by about $1\%-2\%$ from its equilibrium value. We also see that, even though the non-self-consistent results provide a good estimate to the self-consistent ones, full self-consistency is needed in the nonequilibrium case, even for a homogeneous gas. The error bars in the self-consistent results are estimated by comparing the exact exchange energy in equilibrium with the exchange energy obtained from our code for $n_L=n_R$ and different values of $r_x$. Therefore, the exchange energy depends on the current density, but this dependence is extremely weak in our model system. One
could now proceed to calculate this current density explicitly and work out a current dependent local density approximation from the dependence of $E_v$ on the current density. However, the weak dependence of the exchange energy on the current density deduced from Fig. 3 means that the current dependence of the local exchange functional is also very weak, and the changes it will induce in the associated LDA–Kohn-Sham effective potential will be well within the error bar of the LDA itself.

**D. Local exchange potential**

The weak dependence of the local exchange potential on the current density can be seen clearly in terms of the symmetries of the exchange hole. Consider the expression for Slater’s exchange potential, $v_s^x$, in terms of the Hartree-Fock pair distribution function:

$$ v_s^x(r) = \int d^2r g(r-r') - 1 
| r-r' | n(r'), \quad (9) $$

where $n(r')$ is the electron density and $g(r-r')$ is the exchange hole. Then, the difference between equilibrium and nonequilibrium exchange potentials is, for our homogeneous system, given by:

$$ \Delta v_s^x = \int d^2r \frac{\Delta g(R)}{|R|}, \quad (10) $$

where $R$ and $\Delta g$ are defined as above. From Eq. (10), it follows that

$$ \Delta g(X,Y) = - \Delta g(Y,X) \Rightarrow \Delta v_s^x = 0, \quad (11) $$

and hence, only the symmetric part of $\Delta g(X,Y)$ contributes to the deviation of exchange potential with respect to its equilibrium value. Note that $\Delta g(X,Y)$ is an oscillatory function that integrates to zero, which also has a marked antisymmetric character shown in Fig. 1(b). This explains the weak dependence of $E_v$ and $v_s$ on the current density.

**IV. CONCLUSIONS**

In conclusion, we have maximized the entropy of a two-dimensional homogeneous electron gas with constraints on the average total energy and average numbers of left- and right-moving electrons to obtain a simplified description of the steady state within the Hartree-Fock approximation. Our results show that both the single-particle spectrum and the exchange hole depend significantly on the current density, while averaged quantities such as the local exchange potential or the exchange energy do not. Our results provide support to the idea that within a static-DFT approach to quantum transport problems, nonequilibrium corrections to the exchange-correlation functional—at least at the exchange-only level—may be neglected without substantial loss of accuracy.

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That is, to find the Slater determinant that minimizes the expectation value of the effective Hamiltonian $\hat{\mathcal{F}} = \hat{H}_{HF} - \mu_L \hat{N}_R - \mu_R \hat{N}_L$.

For two Fermi hemispheres of radii $k_L$ and $k_R$, the noninteracting electronic current is related to these densities by the expression

$$j = \frac{2}{\pi \epsilon^2} (n_L + n_R) (n_L^3 - n_R^3).$$

In particular, Eq. (22) of Ref. 13 applies also to our considerations here, where $\delta H_{LR}$ contains contributions from the Fock operator that do not vanish for any finite length of the central region.

We may view our two-dimensional electron gas as a simple model of one of the leads to which the nanoscale conductor is attached.