

Nonconservative generalized current-induced forces

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A recent result for the curl of forces on ions under steady-state current in atomic wires with noninteracting electrons is extended to generalized forces on classical degrees of freedom in the presence of mean-field electron-electron screening. Current is described within a generic multiterminal picture, forces within the Ehrenfest approximation, and screening within an adiabatic, but not necessarily spatially local, mean-field picture.

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I. INTRODUCTION

Electrical current flow exerts forces on the atoms in a conductor, in the same way in which a river pushes rocks in its way. While their formal description requires a careful definition, it has long been clear that these forces lie at the heart of a class of phenomena, known as electromigration: the current-driven motion and flow of atoms in a conductor.¹ Nonetheless, a fundamental question about these forces was, until recently, not entirely clear: are they conservative or not, with arguments both ways.¹⁻⁴ The interest in these forces is partly physical and partly practical: in nanoscale conductors, where the current densities can be huge, these forces can, correspondingly, be large, opening up the question of how these corrections to ordinary interatomic forces affect the structure and functionality of atomic-scale devices.⁵⁻⁷

Recently it was shown that current-induced forces are, indeed, not conservative, by evaluating explicitly their curl under steady-state conditions,⁸ and that, therefore, these forces can do net work on the atoms around closed paths. This finding is of interest^{9,10} for several reasons. First, as was shown in Ref. 8, the nonconservative forces constitute the basis for a current-driven atomic-scale motor. Second, the work done by these forces constitutes a new mechanism for energy transfer from current-carrying electrons into the atomic motion, whose implications for phenomena such as electromigration^{11,12} and local heating^{13,14} in nanowires, and for the stability of these systems under current, define a fresh direction for research, with work currently under way.

However, the arguments in Ref. 8 were for noninteracting electrons. The purpose of this paper is to extend the analytical result for the curl of the steady-state force on an ion in a current-carrying nanowire to arbitrary generalized degrees of freedom and to situations with mean-field electron-electron interactions. To this end, we will also extend the multiple-probe open-boundary method in Ref. 15 to multiple electrodes. We illustrate the self-consistent result for the curl with a model example, which shows that while screening reduces the curl, it does not, in general, eliminate it altogether.

Section II defines forces for the purposes of the present discussion. Section III introduces the multiple-lead self-consistent steady state. Section IV makes the above exten-

sions to the curl formula. The model example is in Sec. V and we conclude with a summary in Sec. VI.

II. DEFINITION OF FORCES

For our present purposes, we describe electron-ion interactions at the level of the Ehrenfest approximation. In this approximation, electrons are treated quantum mechanically, while ions are treated as classical point particles, with coordinates $\{R_I\}$, where $I \equiv n\nu$ denotes an ion, n , and a direction, ν . We denote the classical coordinates collectively by

$$R \equiv \{R_I\}. \quad (1)$$

Electrons evolve according to the time-dependent Schrödinger equation, within a mean-field one-electron picture of electron-electron interactions, defined by the following specifications. It will be convenient to work with a discrete orthonormal real-space basis, $\{|i\rangle\}$, such as a computational grid or an orthogonal tight-binding model,^{16,17}

$$\langle i|j\rangle = \delta_{ij}. \quad (2)$$

Electron spin can be included by treating $i \equiv l\sigma$ as a composite index, where l labels a lattice site (or atomic orbital) and σ labels the spin state at that site (orbital). We then assume that electrons, either in a time-dependent or in a steady-state situation, see a one-electron Hamiltonian, \hat{H} , composed of two parts,

$$\hat{H} = \hat{H}(\hat{\rho}, R) = \hat{h}(R) + \hat{v}(\hat{\rho}, R). \quad (3)$$

Here, $\hat{h}(R)$ describes noninteracting electrons, interacting with the classical degrees of freedom R via the electron-ion interaction. $\hat{v}(\hat{\rho}, R)$ is a Hermitian mean-field one-electron potential, about which we assume that it is derived from some model functional, $\mathcal{E}(\hat{\rho}, R)$, of the instantaneous one-electron density matrix (DM) $\hat{\rho}$ via the prescription

$$v_{ij} = v_{ij}(\hat{\rho}, R) = \partial_{ji} \mathcal{E}(\hat{\rho}, R), \quad \partial_{ji} \equiv \frac{\partial}{\partial \rho_{ji}}, \quad (4)$$

where $A_{ij} = \langle i|\hat{A}|j\rangle$ for a one-electron operator \hat{A} . We may assume, for generality, that H_{ij} is not diagonal in the spin

index σ . The explicit dependence of $\mathcal{E}(\hat{\rho}, R)$ on R may arise with anchored basis sets^{16,17} and is allowed here for generality.

A convenient way to obtain the desired quantum-classical description is to start from a suitable quantum-classical Lagrangian.^{16,17} Then the ions evolve under Newtonian equations of motion, with forces, due to the interaction with the electrons, given by

$$F_I = \text{Tr}\{\hat{f}_I(R)\hat{\rho}\} - \partial_I \mathcal{E}(\hat{\rho}, R), \quad (5)$$

where

$$\hat{f}_I(R) = -\partial_I \hat{h}(R), \quad \partial_I \equiv \frac{\partial}{\partial R_I}. \quad (6)$$

This mixed quantum-classical description constitutes a mean-field treatment of electron-ion interactions, which suppresses both quantum-mechanical effects in the motion of ions and electron-ion correlations. This suppression results in known limitations of Ehrenfest dynamics, namely, that it suppresses the spontaneous deexcitation of electrons by exciting phonons. Thus, for example, Ehrenfest dynamics is not suitable for a description of Joule heating.¹⁸ In the context of nonconservative forces under current, however, these limitations are not fatal for reasons discussed in Ref. 8: the rate of work by the nonconservative forces and the rates of dissipation due to inelastic scattering scale differently with atomic mass, and in the limit of heavy ions the former dominates. Thus, for our present purposes we adopt the Ehrenfest picture of electron-ion interactions.

Physically, Ehrenfest dynamics becomes correct in the limit of sufficiently massive or energetic ions. If the underlying quantum-mechanical ionic probability density is sufficiently narrow, then the classical coordinates and forces in Ehrenfest dynamics can be thought of as describing approximately the motion of the centroid of this probability density over restricted time scales.

III. CURRENT-CARRYING STEADY STATE

We now consider current-carrying nanostructures under steady-state conditions, with the aid of the setup in Fig. 1. It shows a central region, C , connected to two or more electrodes or leads labeled by an index α . We will think of the leads as being finite though possibly long. We will use label S to refer collectively to the system composed of these components,

$$S \equiv C \cup \{\alpha\}. \quad (7)$$

To open the system to electron baths, we follow the construction in Ref. 15 and imagine that each site in S is weakly coupled, through a matrix element γ , to an external probe with an energy-independent surface density of states d and a retarded surface Green's function $g^+ = -i\pi d$. Probes coupled to lead α are maintained at electrochemical potential μ_α , with a corresponding Fermi-Dirac distribution $f_\alpha(E)$, and probes coupled to C are maintained at electrochemical potential μ_C , with a corresponding Fermi-Dirac distribution $f_C(E)$. We will denote the collection of electrochemical po-

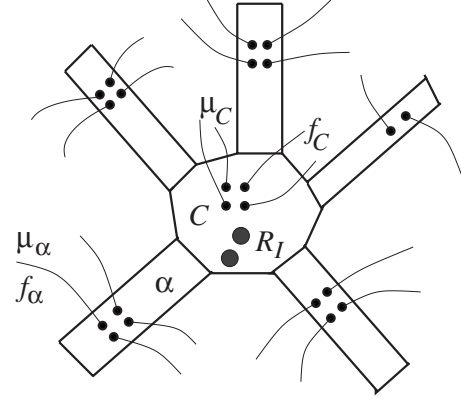


FIG. 1. The setup used to generate a current-carrying steady state in a nanostructure, C , between a set of electrochemically biased electrodes, $\{\alpha\}$. The details are discussed in the text.

tentials and corresponding Fermi-Dirac distributions by

$$\mu \equiv (\mu_C, \{\mu_\alpha\}), \quad f \equiv (f_C, \{f_\alpha\}). \quad (8)$$

Then, either by solving the Lippmann-Schwinger equation for stationary wave functions originating from the external probes and propagating through the system or, equivalently, by the method of nonequilibrium Green's functions, the steady-state one-electron DM in S is given by

$$\hat{\rho}_S = \int_{-\infty}^{+\infty} \hat{\rho}_S(E) dE, \quad \hat{\rho}_S(E) = \hat{G}_S^+(E) \hat{\Sigma}^<(E) \hat{G}_S^-(E), \quad (9)$$

where

$$\hat{G}_S^\pm(E) = [(E \pm i\epsilon)\hat{P}_S - \hat{H}_S]^{-1}, \quad \epsilon = \pi\gamma^2 d \quad (10)$$

are the retarded and advanced Green's functions for S and¹⁹

$$\hat{\Sigma}^<(E) = \frac{\epsilon}{\pi} f_C(E) \hat{P}_C + \frac{\epsilon}{\pi} \sum_\alpha f_\alpha(E) \hat{P}_\alpha. \quad (11)$$

Above, \hat{H}_S is the one-electron Hamiltonian in S , and we have introduced the projection operators

$$\hat{P}_q = \sum_{i \in q} |i\rangle\langle i|, \quad q = C, \{\alpha\}, \quad (12)$$

with

$$\hat{P}_S = \hat{P}_C + \sum_\alpha \hat{P}_\alpha. \quad (13)$$

\hat{H}_S is understood to be self-consistent in the sense $\hat{H}_S = \hat{H}_S(\hat{\rho}, R)$, with the functional $\hat{H}(\hat{\rho}, R)$ defined in Eq. (3). It will be convenient to write Eq. (9) as

$$\hat{\rho}_S(E) = f_C(E) \hat{D}_C(E) + \sum_\alpha f_\alpha(E) \hat{D}_\alpha(E), \quad (14)$$

where

$$\hat{D}_q(E) = \frac{\epsilon}{\pi} \hat{G}_S^+(E) \hat{P}_q \hat{G}_S^-(E), \quad q = C, \{\alpha\}, \quad (15)$$

with

$$\hat{D}_C(E) + \sum_{\alpha} \hat{D}_{\alpha}(E) = \frac{\hat{G}_S^{-}(E) - \hat{G}_S^{+}(E)}{2\pi i} \equiv \hat{D}_S(E). \quad (16)$$

In the last equation, $\hat{D}_S(E)$ is the density-of-states operator for system S , embedded in the sea of external probes.

For any finite ϵ and lead length, this construction gives an approximation to the usual Landauer-Büttiker setup, with infinitely long leads. This approximation, however, is in itself a perfectly admissible transport steady state. In this picture, the sea of external probes, which sets the collection of electrochemical potentials μ , plays the role of an extended nonequilibrium environment, undergoing a long-lived process of equilibration through the finite system S . It is shown in the Appendix how the usual picture, with infinitely long leads, can be recovered from the present setup as a limiting case.

To obtain a well-defined problem, we now make one further stipulation, namely, that the model DM functional \mathcal{E} depends only on $\hat{\rho}_S$ (for a given R) and not on the DM in the extended environment: $\mathcal{E} = \mathcal{E}(\hat{\rho}_S, R)$. This stipulation enables us to treat \mathcal{E} as a well-defined finite quantity. The self-consistent part of the Hamiltonian \hat{H} , \hat{v} , is now restricted to and depends solely on the DM in S : $v_{ij} = v_{ij}(\hat{\rho}_S, R)$; $v_{ij} \neq 0$ only if $i \in S$ and $j \in S$. While this makes the problem, in principle, soluble exactly, it eliminates screening effects in the extended environment outside S : there are no self-consistent adjustments to the one-electron potential in the environment, and both μ and f are independent of the electron-electron interactions in S . This limitation can be questioned on fundamental grounds.²⁰ However, our ansatz does retain certain key effects: the formation of self-consistent resistivity dipoles across scattering centers in S and, in particular, in C , under current, as well as long-range self-consistent potential shifts within the leads $\{\alpha\}$.

In the model of steady-state conduction thus obtained, the self-consistent steady-state DM in S is, ultimately, a function of the inputs R and μ , $\hat{\rho}_S = \hat{\rho}_S(R, \mu)$. By placing this DM in Eq. (5), we obtain the steady-state force exerted on degree of freedom I by the current-carrying electrons²¹

$$F_I = F_I(R, \mu) = \text{Tr}\{\hat{f}_I(R)\hat{\rho}_S(R, \mu)\} - \partial_I \mathcal{E}(\hat{\rho}_S, R)|_{\hat{\rho}_S = \hat{\rho}_S(R, \mu)}. \quad (17)$$

Here, we have made the further assumption that \hat{f}_I is sufficiently short ranged for the first term in Eq. (17) to invoke only the DM in S . However, this assumption is not restrictive as, physically, $\hat{h}(R)$ is short ranged in real space.

The limitations of the above mean-field picture of electron-ion and electron-electron interactions are not a subject of this paper. Instead, here we consider the properties of the steady-state force $F_I(R, \mu)$, thus obtained, and, in particular, the question of whether or not this force is conservative. Although we will continue to speak of ions, the discussion applies to arbitrary classical degrees of freedom $\{I\}$, with generalized coordinates $\{R_{jI}\}$, provided that the corresponding generalized forces can be expressed by Eq. (17). We observe also that Eq. (17) does not make a decomposition of the force into direct and wind components.¹

IV. CURL OF THE FORCE

In Ref. 8, it was shown that current-induced forces are not conservative by examining the curl of the force on an ion in the two-terminal Landauer steady state for noninteracting electrons. Our task now is to do the same within the present multiple-terminal self-consistent picture. We will need several preliminary results.

First, we note that, with $\hat{\rho}_S = \hat{\rho}_S(R, \mu)$, the self-consistent steady-state Hamiltonian in S is also, ultimately, a function of R and μ ,

$$\hat{H}_S = \hat{H}_S(R, \mu) = \hat{H}_S[\hat{\rho}_S(R, \mu), R], \quad (18)$$

and we define the screened force operator

$$\hat{F}_I = \hat{F}_I(R, \mu) = -\partial_I \hat{H}_S(R, \mu) = -\partial_I \hat{h}(R) - \partial_I \hat{v}(R, \mu), \quad (19)$$

where $\hat{v}(R, \mu) = \hat{v}[\hat{\rho}_S(R, \mu), R]$. \hat{F}_I measures the total change in the self-consistent Hamiltonian upon varying degree of freedom I . Next, by use of the Dyson equation, for $\hat{\rho}_S(E) = \hat{\rho}_S(R, \mu, E)$ from Eq. (9) we have

$$-\partial_I \hat{\rho}_S(E) = \hat{G}_S^{+}(E) \hat{F}_I \hat{\rho}_S(E) + \hat{\rho}_S(E) \hat{F}_I \hat{G}_S^{-}(E). \quad (20)$$

Next, we consider the second term in Eq. (17), call it $\Delta F_I(R, \mu)$,

$$-\Delta F_I(R, \mu) = \partial_I \mathcal{E}(\hat{\rho}_S, R)|_{\hat{\rho}_S = \hat{\rho}_S(R, \mu)}. \quad (21)$$

We have

$$\begin{aligned} -\partial_J \Delta F_I(R, \mu) &= \partial_J \partial_I \mathcal{E}(\hat{\rho}_S, R)|_{\hat{\rho}_S = \hat{\rho}_S(R, \mu)} \\ &+ \sum_{i,j} \partial_{ij} \partial_I \mathcal{E}(\hat{\rho}_S, R)|_{\hat{\rho}_S = \hat{\rho}_S(R, \mu)} \partial_J \rho_{S_{ij}}(R, \mu) \\ &= \partial_J \partial_I \mathcal{E}(\hat{\rho}_S, R)|_{\hat{\rho}_S = \hat{\rho}_S(R, \mu)} \\ &+ \sum_{i,j} \partial_I v_{ji}(\hat{\rho}_S, R)|_{\hat{\rho}_S = \hat{\rho}_S(R, \mu)} \partial_J \rho_{S_{ij}}(R, \mu). \end{aligned} \quad (22)$$

Finally, for $v_{ji}(R, \mu) = v_{ji}[\hat{\rho}_S(R, \mu), R]$ we have

$$\begin{aligned} \partial_I v_{ji}(R, \mu) &= \partial_I v_{ji}(\hat{\rho}_S, R)|_{\hat{\rho}_S = \hat{\rho}_S(R, \mu)} \\ &+ \sum_{k,l} \partial_{kl} v_{ji}(\hat{\rho}_S, R)|_{\hat{\rho}_S = \hat{\rho}_S(R, \mu)} \partial_{I \rho_{S_{kl}}}(R, \mu) \\ &= \partial_I v_{ji}(\hat{\rho}_S, R)|_{\hat{\rho}_S = \hat{\rho}_S(R, \mu)} \\ &+ \sum_{k,l} \partial_{kl} \partial_{ij} \mathcal{E}(\hat{\rho}_S, R)|_{\hat{\rho}_S = \hat{\rho}_S(R, \mu)} \partial_I \rho_{S_{kl}}(R, \mu). \end{aligned} \quad (23)$$

Putting these results together, we obtain

$$\begin{aligned} \eta_{IJ} &= \partial_I F_J(R, \mu) - \partial_J F_I(R, \mu) \\ &= \int_{-\infty}^{+\infty} \eta_{IJ}(E) dE, \quad \eta_{IJ}(E) \\ &= 4\pi \text{Im} \text{Tr}\{\hat{F}_I \hat{D}_S(E) \hat{F}_J \hat{\rho}_S(E)\}, \end{aligned} \quad (24)$$

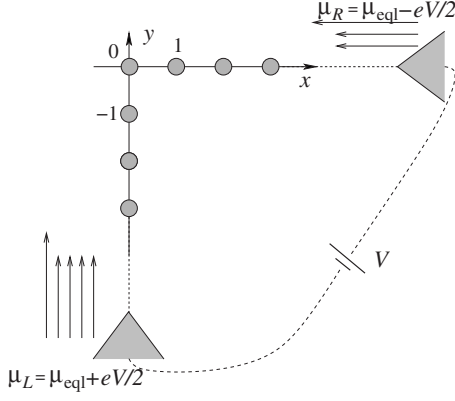


FIG. 2. The two-terminal geometry for the example in the text.

where the density-of-states operator $\hat{D}_S(E)$ was introduced in Eq. (16). Equation (24) is our central result. It extends the earlier finding in Ref. 8 to the present multiple-terminal self-consistent steady state. The key difference is the replacement of the bare force operator \hat{f}_I in the curl expression by the screened force operator \hat{F}_I .

At equilibrium, $\mu_q = \mu_{\text{eq}}$, $f_q(E) = f_{\text{eq}}(E)$, $q = C, \{\alpha\}$. Then $\hat{\rho}_S(E) = f_{\text{eq}}(E)\hat{D}_S(E)$ from Eq. (14), and η_{IJ} vanishes identically. This is a reflection of the fact that forces at equilibrium are conservative. For small departures from equilibrium, the curl expression can be linearized as follows. We set $\mu_C = \mu_{\text{eq}}$, $\mu_\alpha = \mu_C + \Delta\mu_\alpha$ and consider zero electronic temperature when the Fermi-Dirac distribution is a step function. Then

$$\eta_{IJ} = 4\pi \text{Im} \text{Tr}\{\hat{F}_I \hat{D}_S(\mu_{\text{eq}}) \hat{F}_J \Delta\hat{\rho}_S\}, \quad \Delta\hat{\rho}_S = \sum_\alpha \Delta\mu_\alpha \hat{D}_\alpha(\mu_{\text{eq}}), \quad (25)$$

with all quantities now evaluated for the self-consistent equilibrium system.

The conclusion, as in the case of noninteracting electrons, is that, since η_{IJ} does not vanish identically, forces in the multiterminal self-consistent steady state above are, in general, not conservative.

V. EXAMPLE

For our example, we revisit the geometry considered in Ref. 8: an atomic chain with a bend, shown in Fig. 2. Our aims are to calculate the curl of the force on the corner atom, labeled 0, without and with self-consistency, and compare the two results.

The chain is infinite and perfect. The bend angle is 90° . We adopt a spin-degenerate single-orbital nearest-neighbor orthogonal tight-binding model with a hopping integral $H < 0$. Below, $|l\rangle$ will denote the orbital basis state at site l in the chain. Operators will be spinless, and a spin-degeneracy factor of 2 will be included in the final results.

The two electrochemical potentials for the two-terminal assembly are $\mu_{L,R} = \mu_{\text{eq}} \pm eV/2$, where μ_{eq} sets the band filling ν in the perfect chain, with $\nu = 1$ corresponding to a com-

pletely filled band. Self-consistency takes the form of local charge neutrality, imposed on the corner atom only. The only parameter, varied to achieve self-consistency, is the onsite energy, E_0 , on the corner atom. When the corner atom is in its ideal position, all onsite energies are equal and set to zero. This model corresponds to the functional $\mathcal{E}(\hat{\rho}) = U(\langle 0|\hat{\rho}|0\rangle - \nu)^2/2$ in the limit $U \rightarrow \infty$.

With the choice of axes in Fig. 2, for the corner atom in the ideal position we have

$$\hat{F}_x = H'(|0\rangle\langle 1| + |1\rangle\langle 0|) + |0\rangle\zeta\langle 0|, \quad (26)$$

$$\hat{F}_y = -H'(|0\rangle\langle -1| + |-1\rangle\langle 0|) - |0\rangle\zeta\langle 0|. \quad (27)$$

The terms in parentheses in each equation give the bare force operator, the second term in each case is the self-consistent part of the screened force operator, and H' denotes the derivative of the hopping integral with distance. To evaluate ζ , we imagine displacing the corner atom through a small amount δy along y and require it to acquire an onsite energy shift δE_0 , such as to prevent the atom from acquiring any extra charge, whereupon $\zeta = \delta E_0 / \delta y$. To proceed further, we specialize to the small-bias regime in Eq. (25). Then, invoking linear response theory, ζ is given by the condition

$$\oint_c \langle 0|\hat{G}(z)\hat{F}_y\hat{G}(z)|0\rangle dz = 0, \quad (28)$$

where $\hat{G}(z)$ is the Green's function for an infinite perfect chain and the simple-closed contour c cuts the real energy axis at μ_{eq} and at a second energy, below the bottom of the band ($-2|H|$). For $\text{Im} z > 0$, $\hat{G}(z)$ is given by

$$\langle k|\hat{G}(z)|l\rangle = \frac{\left(\frac{z - \sqrt{z^2 - 4H^2}}{2H}\right)^{|l-k|}}{\sqrt{z^2 - 4H^2}}, \quad (29)$$

where the square root is defined by $\sqrt{r^2 e^{2i\theta}} = r e^{i\theta}$, $r > 0$, $0 < \theta < \pi$. At other energies, the Green's function is obtained from $\hat{G}(z^*) = \hat{G}^\dagger(z)$. Then

$$\zeta = -2H' \left(1 - \frac{2\phi}{\pi}\right), \quad (30)$$

where ϕ is related to μ_{eq} through $\mu_{\text{eq}} = 2H \cos \phi$ and to the band filling through $\nu = \phi/\pi$.

The operators $\hat{D}_\alpha(\mu_{\text{eq}})$ in Eq. (25) are now given by

$$\langle k|\hat{D}_{L,R}(\mu_{\text{eq}})|l\rangle = -\frac{1}{2\pi 2H} \frac{e^{\pm i(k-l)\phi}}{\sin \phi}. \quad (31)$$

Then for the curl of the force on the corner atom, in the small-bias limit [Eq. (25)], in the non-self-consistent case ($\zeta = 0$), we obtain, including a spin-degeneracy factor of 2,

$$\eta_{xy}^{\text{nsc}} = \frac{4eV H'^2 \cos \phi}{\pi H^2 \sin \phi}, \quad (32)$$

while in the self-consistent case we find²²

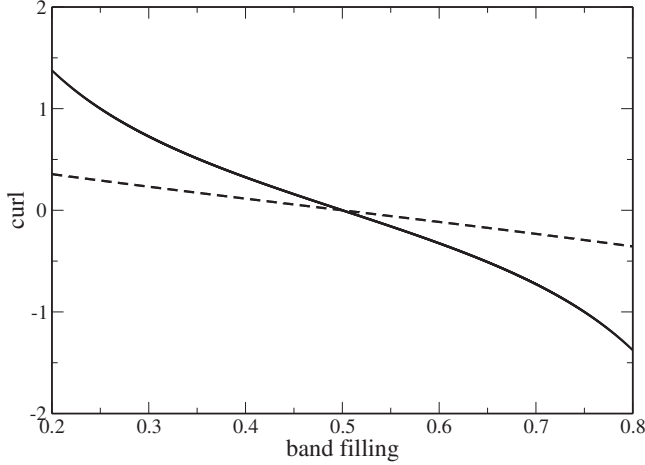


FIG. 3. η_{xy}^{nc} (solid line) and η_{xy}^{sc} (dashed line), in units of $(4eV/\pi)(H'^2/H^2)$, versus band filling, for the corner atom in the geometry in Fig. 2.

$$\eta_{xy}^{\text{sc}} = \frac{4eVH'^2}{\pi H^2} \frac{1}{\sin \phi} \left(\cos \phi - 1 + \frac{2\phi}{\pi} \right). \quad (33)$$

These results are plotted in Fig. 3. Both vanish for a half-filled band ($\phi = \pi/2$). For fractional band fillings, in the region, say, $\nu \sim 1/3$, $\eta_{xy}^{\text{sc}}/\eta_{xy}^{\text{nc}} \sim 1/3$. Thus, screening reduces the curl considerably, but it does not eliminate it altogether.

VI. SUMMARY

In this paper, the result for the curl of current-induced forces under steady-state transport from Ref. 8 has been extended in three ways: we have considered a general multiterminal assembly, a general one-electron self-consistent description of screening, and we have kept the discussion sufficiently general, to make the results applicable to arbitrary classical degrees of freedom, interacting with the current-carrying electrons. An example of such generalized coordinates are magnetic degrees of freedom in spin-polarized nanowires.⁴ The key finding [Eq. (24)] is that the generalized self-consistent steady-state forces remain, in general, nonconservative. The example of Sec. V shows that while screening can reduce the curl considerably, there still is a nontrivial amount left over.

It is hoped that the general results in Eqs. (24) and (25) will be of use to other researchers in investigating and analyzing current-induced generalized forces and the problem of their (non-)conservative nature. An interesting question is what happens to the screened curl in situations where strict local charge neutrality is imposed on more and more atoms and, specifically, in the limit where it is imposed on all infinitely many atoms.³ This question, as well as dynamical simulations of the atomic motion under self-consistent non-conservative forces, is left for future work.

A further question for future research is what happens beyond mean-field electron-electron interactions. Here we merely observe that Sorbello's original thought experiment,¹ to argue that current-induced forces must be nonconservative, applies to noninteracting and interacting electrons alike.

Therefore, we do not expect our present conclusions to change in a qualitative way when corrections to the mean-field description are included.

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APPENDIX

Our task here is to relate the construction of Sec. III to the usual Landauer-Büttiker picture, with semi-infinite leads. This can be done by a limiting process¹⁵ as follows. It will be convenient to partition \hat{H}_S as

$$\hat{H}_S = \hat{H}_0 + \hat{V}, \quad (A1)$$

where

$$\hat{H}_0 = \hat{H}_C + \sum_{\alpha} \hat{H}_{\alpha}, \quad \hat{H}_q = \hat{P}_q \hat{H}_S \hat{P}_q, \quad q = C, \{\alpha\}, \quad (A2)$$

$$\hat{V} = \sum_{\alpha} (\hat{H}_{\alpha C} + \hat{H}_{C\alpha}), \quad \hat{H}_{\alpha C} = \hat{P}_{\alpha} \hat{H}_S \hat{P}_C = \hat{H}_{C\alpha}^{\dagger}. \quad (A3)$$

Here, we have assumed that the Hamiltonian \hat{H}_S does not contain direct lead-to-lead couplings. Let us define

$$\hat{g}_S^{\pm}(E) = [(E \pm i\epsilon)\hat{P}_S - \hat{H}_0]^{-1} = g_C^{\pm}(E) + \sum_{\alpha} g_{\alpha}^{\pm}(E), \quad (A4)$$

where

$$\hat{g}_q^{\pm}(E) = [(E \pm i\epsilon)\hat{P}_q - \hat{H}_q]^{-1}, \quad q = C, \{\alpha\}. \quad (A5)$$

Let us also define

$$\hat{d}_q(E) = \frac{\hat{g}_q^{-}(E) - \hat{g}_q^{+}(E)}{2\pi i} = \frac{\epsilon}{\pi} \hat{g}_q^{+}(E) \hat{P}_q \hat{g}_q^{-}(E), \quad q = C, \{\alpha\}. \quad (A6)$$

Above, $\hat{g}_q^{\pm}(E)$ are the retarded and advanced Green's functions for component q coupled to its external probes but not coupled to any other components and $\hat{d}_q(E)$ is the density-of-states operator for component q in that situation.

$\hat{G}_S^{\pm}(E)$ and $\hat{g}_S^{\pm}(E)$ are linked by the Dyson equation,

$$\hat{G}_S^{\pm}(E) = \hat{g}_S^{\pm}(E) + \hat{g}_S^{\pm}(E) \hat{V} \hat{G}_S^{\pm}(E) = \hat{g}_S^{\pm}(E) + \hat{G}_S^{\pm}(E) \hat{V} \hat{g}_S^{\pm}(E). \quad (A7)$$

With the aid of this equation and the above definitions, we have

$$\hat{D}_q(E) = [\hat{P}_S + \hat{G}_S^{+}(E) \hat{V}] \hat{d}_q(E) [\hat{V} \hat{G}_S^{-}(E) + \hat{P}_S], \quad q = C, \{\alpha\}. \quad (A8)$$

For the DM in C we then find

$$\hat{\rho}_C(E) = \hat{P}_C \hat{\rho}(E) \hat{P}_C = \hat{G}_C^+(E) \hat{\sigma}^<(E) \hat{G}_C^-(E) + [\hat{P}_C + \hat{G}_C^+(E) \hat{\sigma}^+(E)] \hat{\rho}_{0,C}(E) [\hat{\sigma}^-(E) \hat{G}_C^-(E) + \hat{P}_C], \quad (\text{A9})$$

$$\hat{\rho}_{0,C}(E) = f_C(E) \hat{d}_C(E). \quad (\text{A13})$$

where

$$\hat{\sigma}^<(E) = \sum_{\alpha} f_{\alpha}(E) \hat{H}_{C\alpha} \hat{d}_{\alpha}(E) \hat{H}_{\alpha C}, \quad (\text{A10})$$

$$\hat{G}_C^{\pm}(E) = [(E \pm i\epsilon) \hat{P}_C - \hat{H}_C - \hat{\sigma}^{\pm}(E)]^{-1}, \quad (\text{A11})$$

$$\hat{\sigma}^{\pm}(E) = \sum_{\alpha} \hat{H}_{C\alpha} \hat{g}_{\alpha}^{\pm}(E) \hat{H}_{\alpha C}, \quad (\text{A12})$$

Consider now the limit where the lead length becomes infinite and ϵ vanishes while always remaining much larger than the typical electron energy-level spacing in the leads. Then matrix elements of $\hat{g}_{\alpha}^{\pm}(E)$ between real-space basis states that are a finite distance apart tend to those for a truly semi-infinite lead. In this limit, further, $\hat{d}_C(E)$ becomes $\hat{d}_C(E) = \sum_C |C\rangle \delta(E - E_C) \langle C|$, where $\{|C\rangle\}$ are the eigenstates of \hat{H}_C , with eigenenergies $\{E_C\}$. Then Eq. (A9) turns into the expected result for a finite sample (C), embedded between semi-infinite electrodes.

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