Are current-induced forces conservative?

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Abstract

The expression for the force on an ion in the presence of current can be derived from first principles without any assumption about its conservative character. However, energy functionals have been constructed that indicate that this force can be written as the derivative of a potential function. On the other hand, there exist compelling specific arguments that strongly suggest the contrary. We propose physical mechanisms that invalidate such arguments and demonstrate their existence with first-principles calculations. While our results do not constitute a formal resolution to the fundamental question of whether current-induced forces are conservative, they represent a substantial step forward in this direction.

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Electrons flowing in a conductor can transfer momentum to the ions. From a static point of view, the steady-state electron density in a current-carrying conductor is microscopically different from that in the absence of current. In either picture, the passage of current generates additional forces on ions. This may result in atomic rearrangements and diffusion of atoms, a phenomenon known as electromigration. The advent of microelectronics has sparked off a considerable interest in electromigration since it has been found to be a major failure mechanism in metallic interconnects. In recent years, a new type of electronics is being considered which envisions the use of nanoscale components. Since nanoscale conductors can carry current densities much larger than their macroscopic counterparts, the problem of electromigration is again of key importance. Recent work has studied the effect of current-induced forces in atomic and molecular wires and nanoscale conductors. Combined with early investigations on the subject, this work has shed new light on the microscopic mechanism of current-induced mechanical effects.

While a consensus on the physical origin of current-induced forces seems to have been reached, a fundamental question remains unanswered: are current-induced forces conservative? The difficulty in answering this question is intimately related to the difficulty in defining a force in a non-equilibrium problem.

In this paper we address this question in the following way: we consider representative arguments against the conservative nature of current-induced forces and suggest physical mechanisms that invalidate these arguments. We then corroborate the existence of such mechanisms with first-principles calculations. While this by no means proves that these forces are conservative, we believe it is a substantial step forward in this direction and hope that our suggestions will generate much-needed discussions.

Let us start from the expression for forces in the presence of current. This expression can be derived in different ways. One approach is to start from a fully dynamical quantum description of the many-body problem comprising electrons and ions, and then take the limit as the ionic motion becomes classical. In this derivation, the force expression comes about as the classical limit of Ehrenfest’s theorem applied to the rate of change of the momentum of an ion. Formally, this limit corresponds to high ionic masses or high kinetic energies. A different approach is to start from an appropriate mixed quantum-classical Lagrangian. The force expression then results from the Euler-Lagrange equation of motion for the classical ions. Both approaches result in the same expression for the force on a given ion, with position \( \mathbf{r} \), due to the self-consistent electronic density \( \rho(\mathbf{r}) \) under current flow:

\[
F = -\int d\mathbf{r} \frac{\partial v}{\partial \mathbf{r}} \rho(\mathbf{r}),
\]

which can be equivalently written as

\[
F = -\sum_i \langle \psi_i | \frac{\partial v}{\partial \mathbf{R}} | \psi_i \rangle - \lim_{\Delta \to 0} \int dE \langle \psi_\Delta | \frac{\partial v}{\partial \mathbf{R}} | \psi_\Delta \rangle.
\]

where \( v \) is the electron-ion interaction. The first term on the RHS of Eq. (2) is similar to the usual Hellmann-Feynman contribution to the force due to localized electronic states |\( \psi_i \)\). The second term is the contribution to the force due to continuum states. The wavefunctions |\( \psi_\Delta \)\) are eigendifferentials in the continuum \( \sigma \). Due to the algebraic equivalence of the above two equations, in the following, when discussing current-induced forces, we will refer to either one without distinction.

Let us now turn to the question of whether or not these forces are conservative. It is essential to emphasize that the force obtained either from the Ehrenfest’s theorem or a Lagrangian formulation, is not necessarily conservative because the above first-principles dynamical derivations do not contain any assumption about the existence, or otherwise, of a free energy functional, of which this force might be the derivative. However, as a separate exercise, it was suggested both in Ref. [13] and
in Ref. [14] that forces in the presence of current can also be written as derivatives of appropriate energy functionals. For instance, in Ref. [13] the stationarity of an action was used to map the force problem into a variational one in which the force can be written as the derivative of an energy function. In Ref. [14] an entropy function was used, whose maximization (constrained to the energy of the current-carrying system and the numbers of electrons in it that originate from the right and left reservoirs) again yields the force as the derivative of a potential function. These independent derivations suggest that current-induced forces are conservative.

On the other hand, there exist compelling specific arguments that strongly suggest that current-induced forces cannot be conservative. These arguments consist in gedanken experiments, aimed at showing that the work done by current-induced forces along specific closed paths is not zero and that, therefore, these forces are not conservative. Below we refer to one notable such construction due to Sorbello. [1] This example is of charming simplicity and is particularly convincing. The argument goes like this. Picture a single defect atom in a current-carrying wire between bulk electrodes under an applied bias $V$. First, let the atom move, quasi statically, from a point $A$ to a point $B$ inside the wire (see schematic in Fig. 1). The current-induced force on the defect in the wire does some non-zero work on the way. Now imagine taking the atom from $A$ to $B$ along a path that goes outside the wire (see Fig. 1). Since outside the wire there apparently is no current, no current-induced force should be present. Hence, the work done by current-induced forces on the atom along the path from $A$ to $B$ inside the wire cannot be the same as along the path outside the wire. This would be sufficient to prove that current-induced forces are not conservative.

However, there is something missing in this argument: the quantum-mechanical nature of current outside the wire. Let $|\psi\rangle$ be the global current-carrying electron states for the system. If there always is some (however small) quantum-mechanical coupling between the atom and the wire, there will always be some non-zero tunneling probability for electrons to get from the wire onto the atom, and back. The atom then acts as a resonant center and there will always exist an energy window where the states $|\psi\rangle$ contain resonant paths that emerge from the wire, pass through the atom, and go back into the wire. Due to the scattering of electrons at the atom, these resonant paths may be expected to create a charge dipole, centered at the atom, much like the local resistivity dipole in electromigration. [1] Increasing the distance $d$ between the atom and the wire will make the resonant energy window narrower, while the resonance will remain pinned against the energy window $eV$, due to self-consistency. Now, the total current carried by the resonance is given by the energy integral, over the energy window $eV$, of a transmission function, $T(E)$. As the resonance gets narrower in energy, so does $T(E)$. $T(E)$ is always bounded and hence, as $d$ increases, the total current carried by the resonance will decrease.

On the other hand, the charge dipole across the resonant center originates from the density of states, $DOS(E)$, due to the populated current-carrying electron states in the energy window $eV$. By contrast with $T(E)$, $DOS(E)$ is unbounded: if $d$ increases, the resonant peak in $DOS(E)$ gets narrower but taller in such a way that its energy integral remains constant. Since current-induced forces are related to the integral of the density of states [see e.g. Eq. (2)], we expect the force on the atom due to the resonant dipole to be constant with $d$. In other words, there is always a current-induced force on the atom, even outside the wire, and this force does not vanish with increasing $d$.

A key assumption of our reasoning is that there always is some coupling between the atom in the vacuum and the metal. If this coupling is truncated artificially, then the current and the “resonant-dipole force” will both be discontinuously extinguished. However, such a truncation would at the same time create a bound state (at the atom) in the continuum, and would thus modify the nature of the electronic spectrum and of the corresponding Born-Oppenheimer (BO) manifold. Such a discontinuous modification corresponds to a breakdown of the BO approximation, in which case the notion of conservative forces is lost by definition.

Our analysis above relies only on generic properties of resonant transmission. We therefore now seek to demonstrate the existence of a resonant dipole in the simplest possible resonant configuration: that of a single atom in the vacuum between two bulk electrodes. Our goal is to show that this resonant dipole gives rise to a finite current-induced force that does not vanish with increasing electrode separation, even when the current dies out. To this end, we have performed first-principles calculations of the current-induced force on a single Si atom between two jellium electrodes. [14] The interior electron...
density of the electrodes is taken equal to the value for metallic gold \((r_s \approx 3)\). The electrodes are kept at a certain bias with the left electrode positively biased so that electrons flow from right to left. In Fig. 2 we plot the density of states as a function of energy for a bias of 0.1 V and different distances between the jellium edges of the two electrodes. It is clear from this figure that a resonance develops in the energy window between the left and right chemical potentials. The resonance becomes narrower and taller with increasing distance. It is also evident from Fig. 2 that this resonance is pinned towards the right chemical potential. Such pinning can be intuitively understood as follows. By increasing the distance between the electrodes the resonance becomes narrower and narrower. In order to preserve charge neutrality, the amount of charge accommodated by the resonance needs to be the same at all distances. The only way to achieve this is for the “center” of the resonance to move closer to the right electrochemical potential.

Now that we have shown the existence of the resonance, let us look at the spatial distribution of the charge dipole it creates across the atom. In order to do this we follow Lang’s approach and calculate first the difference between the electronic distribution at a given bias \(\rho(r,V)\) and the corresponding distribution at zero bias \(\rho(r,0)\). Call this quantity \(\tilde{\rho}(r,V)\). It contains three contributions: (i) the polarization of the biased electrode-electrode system without the atom, (ii) the polarization of the electron cloud at the atom due to the field generated by (i), and (iii) the current-induced resonant dipole. The first two terms generate a force of equal magnitude but opposite sign so they do not contribute to the total force. (An isolated atom in a uniform electric field does not have a net force on its nucleus). To eliminate (i) and (ii), we subtract (i) from \(\tilde{\rho}(r,V)\) and take the difference between the result of that subtraction at a given electrode-electrode distance and the same quantity at a larger separation scaled to the field of the previous distance. This gives a negative fraction of the current-induced dipole, so a change of sign is necessary. Call this quantity \(\rho_f(r,V)\). Finally, to isolate the antisymmetric (dipole) component of this distribution we evaluate \(\rho_f(r,V) - \rho_f(r,-V)\). The result is plotted in Fig. 3 for a separation of 10 a.u. (with respect to 16 a.u.) and clearly shows the current-induced resonant dipole across the atom. The dipole has positive charge on the left of the atom and negative charge on its right so that the current-induced force pushes the atom to the right, i.e. against the electron flow.

Finally, we have to show that the current decreases with electrode separation while the force does not. This is plotted in Fig. 4 for different electrode separations. It is clear from Fig. 4 that the current decreases substantially with electrode separation while the force saturates at a value of about 2 mRy/a.u. Notice again that this force is positive, i.e. it pushes the atom against the electron flow, in agreement with the sign of the resonant dipole. These numerical results confirm our conjecture: as long as the atom is coupled to the electrodes, a resonant dipole forms across it, such that a non-zero current-induced force is exerted on the atom that persists with separation even as the current dies out.

We conclude by stressing again that our goal here is to show that existing arguments against the conservativeness of current-induced forces ignore specific physical mechanisms. These mechanisms predict the existence of current-induced forces in unexpected places, such as an atom in the vacuum next to a current-carrying metal. We have demonstrated the existence of such forces using first-principles calculations. These results do not prove that current-induced forces are conservative but we believe that they give extra support in favor of such a con-
It is worth mentioning at this point that the problem is not just "academic", but can have an impact in nanoscale electronics. As an example, consider a perfect, defect-free quasi-two-dimensional wire and identify two points of the wire in such a way that a straight line connecting these points separates the wire in two equivalent regions. If the force is non-conservative, then you can move an atom from one point to the other along different paths in the two equivalent regions such that the work done by the current-induced force is different for the different paths. As a consequence, it is in principle possible to break equivalent regions of a defect-free wire differently. While this effect might not be important in macroscopic wires, it is relevant in nanoscale conductors made of a relatively small number of atoms. A further implication of the problem is the following. If current-induced forces are not conservative, then their cross-derivatives with respect to ionic positions are not necessarily equal and hence the dynamical response matrix for a current-carrying structure is not necessarily symmetric, in which case the conventional notion of phonons would be lost in the presence of current.

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