Steady-state density functional theory for finite bias conductances

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The popular ab-intio framework to describe electron transport combining static density functional theory (DFT) with the Landauer formalism is in principle incomplete since it neglects the dynamical exchange-correlation (xc) contributions to the bias stemming from time-dependent DFT. Unfortunately, modelling of these dynamical xc contribution is still in its infancy.

Here we propose a steady-state DFT formalism with the density on the junction as well as the steady-state current as basic variables. We prove that the map between the set local potential \( v(r) \) and bias \( V \) on one hand and local density \( n(r) \) and steady-state current \( I \) on the other hand is invertible in a finite bias window around \( V=0 \). The resulting Kohn-Sham system features two xc potentials, an xc contribution to the local gate potential and an xc contribution to the bias. We construct these xc potentials for model systems by reverse engineering and show that they exhibit step-like ridges in the plane of total electron number and current. For small currents these ridges emerge as the discontinuity of the equilibrium xc potential at integer electron number bifurcates. These ridges are the crucial feature to describe within a DFT framework the typical Coulomb blockade diamonds in the differential conductance of nanoscale systems in the plane of gate and bias voltages.