Dynamical correction of thermoelectric coefficients for strongly interacting electrons in the Coulomb blockade regime

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Abstract:
For molecules weakly coupled to leads the exact zero-bias Kohn-Sham conductance can be orders of magnitude larger than the true conductance due to the lack of dynamical exchange-correlation effects. Recently, it has been shown [1] how these dynamical exchange-correlation corrections can be calculated using only quantities obtained from static density functional theory. Here we investigate thermoelectric transport and derive the exchange-correlation correction to the Seebeck coefficient. We show how the Coulomb blockade peaks in both the conductance and the Seebeck coefficient correspond to changes of the number of electrons on the molecule by an integer. Finally, we compare our results to some recent experiments.

[1] S. Kurth and G. Stefanucci, Phys. Rev. Lett. **111**, 030601 (2013), Phys. Rev. Lett. **107**, 216401 (2011).