Thermo-electric effects in nanoscale systems out of equilibrium[1]
YONATAN DUBI, ROBERTO D'AGOSTA, MASSIMILIANO DI VENTRA, University of California-San Diego — As technology advances into the nanoscale regime, probing the electronic properties of nanoscale circuits has become a major challenge. Specifically, it has been suggested that thermo-electric effects may serve as a tool to study electronic properties of nanoscale systems, and experiments on thermo-power in quantum point contacts (QPCs) and molecular circuits have been performed. On the theoretical side, however, linear-response theory is inadequate to determine the dynamical formation of the thermo-electric effect. Here, we propose a novel scheme to calculate dynamical thermo-electric effects in nanostructures arbitrarily far from equilibrium using a local generalization of the Lindblad master equation. We demonstrate the method by calculating the charge imbalance of a QPC in the presence of Coulomb interactions and a temperature gradients, and obtain the long-time energy distribution in the QPC out of equilibrium. Our suggested scheme can be implemented into stochastic time-dependent current-density functional theory [PRL, 98, 226403 (2007)], thus providing a valuable tool in studying the interplay of charge and energy currents for arbitrary many-body systems.

Yonatan Dubi
University of California-San Diego

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