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Many-body theory of electric and thermal transport in single-molecule heterojunctions

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Electron transport in single-molecule junctions (SMJ) is a key example of a *strongly-correlated system far from equilibrium*, with myriad potential applications in nanotechnology. When macroscopic leads are attached to a single molecule, a SMJ is formed, transforming the "few-body" molecular problem into a true "many-body" problem. Until recently, a theory of transport that properly accounts for both the particle and wave character of the electron has been lacking, so that the Coulomb blockade and coherent transport regimes were considered "complementary." We have developed a nonequilibrium many-body theory[1] that reproduces the key features of both the Coulomb blockade and coherent transport regimes simultaneously. Our approach is based on nonequilibrium Green's functions, enabling physically motivated approximations that sum terms to all orders. The junction Green's functions are calculated exactly in the sequential-tunneling limit, and the corrections to the electron self-energy due to finite tunneling width are included via Dyson-Keldysh equations. In this talk, I will present a brief overview of our many-body theory of SMJ and discuss the simulated linear and nonlinear response of a benzenedithiol-gold junction. I will also outline our derivation of an exact expression for the heat current in an interacting nanostructure, highlighting our prediction[2] of a dramatic quantum-induced enhancement of thermoelectric effects in the vicinity of a transmission node. Finally, I will provide several striking examples where the predictions of our many-body theory differ drastically from those of mean-field (density functional) theory.

[1]J. P. Bergfield and C. A. Stafford, Phys. Rev. B **79**, 245125 (2009).
[2]J. P. Bergfield and C. A. Stafford, Nano Letters **9**, 3072 (2009).