Transport in Nanoscale Conductors from First Principles

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Electronic transport is a challenging problem when one wants to solve it from first principles. Physical issues that need to be considered include coherence effects, current fluctuations, local heating, current-induced forces, and so on. To complicate matters electric current does not generally satisfy a minimum principle [1].

I will present a theoretical approach that addresses the above issues. The approach is based on the self-consistent solution of the Lippmann-Schwinger equation [2] within the density functional theory of many-electron systems for a sample connected to metallic electrodes with a finite bias. The formalism provides the most fundamental quantities to describe the dynamics of the whole system: the self-consistent electronic wave functions. From these wave functions, all physical quantities of interest can be derived. To exemplify the approach I will present results on coherence effects [3], current-induced forces [4], coupling to low-energy bosons [5], shot noise, [6] and local heating [7] in selected atomic and molecular wires. Work supported in part by NSF, Carilion Biomedical Institute and ACS-Petroleum Research Fund.

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