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Density Functional Theory of the electrical conductivity of molecular devices

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The theoretical modeling of electrical transport through nanoscale devices is a very challenging task: On one hand, the conduction properties of a molecular junction depend crucially on details of the chemical bonding, particularly at the interface. Such properties are routinely studied using methods based on density-functional theory (DFT). On the other hand, ground-state theories like DFT cannot be directly applied to systems with a finite current, because such devices are out of equilibrium. One possibility to overcome this problem is to study electron transport in the time domain. In the spirit of what is done in semiclassical Boltzmann approaches, one considers the system subject to both an external electrical field and to dissipation due to inelastic scattering. The combined influence of the external driving force and dissipation leads to a steady state with finite current. In this presentation I will first show how time-dependent DFT can be formally extended to dissipative systems, described by a Liouville master equation for the reduced density matrix. In a second step this formalism is then applied to calculate the current-voltage characteristics of molecular junctions, like e.g. carbon nanotubes suspended between metallic contacts.