Max-Planck-Institut für Struktur und Dynamik der Materie

Max Planck Institute for the Structure and Dynamics of Matter

Wednesday, June 29th 2016 - 15:30
CFEL Seminar room 1 (Blgd. 99)

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Time-dependent quantum transport in nanosystems: A nonequilibrium Green's function approach

Quantum transport is often discussed in the steady-state regime where the characteristics of the system are described in terms of the energy-dependent transmission or conductance. There is, however, no guarantee that this description would capture the essential physics in, say, atomic-scale junction operating at high frequencies. Therefore, we look for an accurate theory for describing the full time-dependence. The time-dependence also provides us with "transient spectroscopy" which can give detailed information about the nanosystems out of equilibrium. In this talk, a time-dependent extension to the Landauer—Büttiker approach is presented. The nonequilibrium Green's function approach is employed for describing the charge and heat transport dynamics. The importance of the method is that it provides a closed formula for the time-dependent density matrix in both electronic and phononic systems. In the electronic case the nonequilibrium conditions are due to a switch-on of a bias voltage in the leads or a perturbation in the junction whereas in the phononic case the central region is coupled to reservoirs of different temperatures. In both cases the time-dependent density matrices, and other transport properties such as local charge and heat currents, may be evaluated without the necessity of propagating individual single-particle orbitals or Green's functions. Furthermore, several applications with, e.g., graphene-based circuitries are presented and discussed.

Host: Angel Rubio

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