

A new open quantum system approach for the calculation of non-equilibrium transport properties

Ralph Gebauer

*The Abdus Salam International Centre for Theoretical Physics
Trieste, Italy*

A new method for the calculation of transport properties in nanoscale or mesoscopic systems will be presented. In this approach, the system of interest, e.g. a molecule that is comprised between two metallic wires, is modeled using a supercell-geometry in which the molecule together with a finite length of wire is repeated periodically. An external electric field is applied to this system, and the electronic current created by that field is calculated.

However, a current-carrying steady state can only be reached if dissipative effects are included in the model, therefore allowing for a thermalization of the electrons. This is achieved by describing the electrons as an open quantum system which is in contact with an external bath. In this talk it will be explained how both the external electric field and the dissipative effects can be included in a time-dependent calculation, and applications of this method to resonant tunneling devices will be shown.

This work has been done in collaboration with Roberto Car at Princeton University.