Quantum transport in semiconductor nano-heterostructures

by Paul N. Racec

In this talk we review some mathematical challenges and our solutions arising from modeling of semiconductor nanodevices. Often, the active part of a nanodevice is a quantum system to which electrical contacts are attached such that there is an open quantum system on hand. The scattering theory is suitable for describing such systems. A practical method for computing the scattering matrix, even for 2D and 3D systems, is the R-matrix formalism. For this, one solves the Wigner-Eisenbud eigenvalue problem, i.e. the single-band effective mass Schrödinger equation on the scattering region with mixed Dirichlet/Neumann boundary conditions. Using the finite volume method one may take into account even a position dependent effective mass inside the heterostructure. The R-matrix formalism also yields the scattering wave functions inside the scattering region. Applications of this formalism to nanowire heterostructures will be provided.
As a consequence of opening the quantum system its discrete spectrum becomes a continuous spectrum with resonances. The practical computation of resonances as poles of the scattering matrix is also possible within R-matrix formalism. Furthermore, it allows for a systematic expansion in case of interacting resonances. We obtain a qualitative description of the peaks and dips in the linear conductance of a single electron transistor by Fano lines, where the complex asymmetry parameter is computed explicitly.
In order to compute the physical observables, one needs to know the density matrix of the system. The Landauer-Büttiker formalism provides an ansatz for the density matrix for open quantum systems. In the last years, a detailed analysis has been done in our group in order to mathematically justify the above ansatz.
Finally we discuss future challenges of a realistic modeling of semiconductor nanodevices, like many-particle description and dissipative interaction.

This is a joint work with Hans-Christoph Kaiser, Hagen Neidhardt and Roxana Racec.