Quantum transport simulation:
Non-equilibrium Green's function approach

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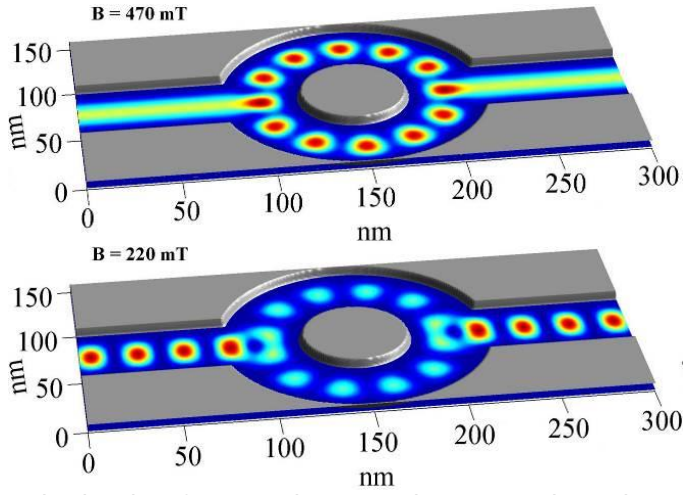
The continuous advancements in the miniaturization techniques have allowed the fabrication of structures with nanometer size. At this scale, quantum physics effects play a significant role and result in spectacular phenomena such as conductance quantization, quantum interference, quantum Hall effect and many others.

In this context, numerical simulations turn out to be a powerful tool for investigating and predicting the electronic transport properties of nanostructures and for exploring their potentiality in view of perspective innovative electronic devices. Among the different possible approaches for simulating electronic transport at the quantum level, the Non-Equilibrium Green's Function (NEGF) method is the most versatile. Indeed, it is able to rigorously treat a variety of important effects at the nanoscale, as non-equilibrium transport, elastic and inelastic scattering and the presence of external magnetic fields.

The goal of this practical work is to **introduce the basics of NEGF technique** and use it to study electron transport through some interesting nanostructures by **numerical simulations**, which will be performed by the students during the class.



Local density-of-states in an Aharonov-Bohm ring at magnetic fields such that a maximum (top panel) or a minimum (bottom panel) of the magnetoconductance occurs.

We will start with a theoretical introduction to illustrate the numerical techniques adopted for calculating the Green's functions of the investigated systems. We will clarify the physical meaning of the self-energy operators and the relation between Green's functions and fundamental physical quantities, as the local density-of-states and the current flow.

Finally, we will simulate typical quasi-one-dimensional structures as quantum nanowires, quantum point contacts and Aharonov-Bohm rings.

Some references for theory and applications:

[1] A. Cresti, G. Grosso and G. Pastori Parravicini, *Theoretical imaging of current profiles in two-dimensional devices*, Eur. Phys. J. B **53**, 537 (2006)

[2] J. Park, K.-H. Xue, M. Mouis, F. Triozon and A. Cresti, *Electron transport properties of mirror twin grain boundaries in molybdenum disulfide: Impact of disorder*, Phys. Rev. B **100**, 235403 (2019)

[3] A. Cresti, *Convenient Peierls phase choice for periodic atomistic systems under magnetic field*, Phys. Rev. B **103**, 045402 (2021)

Profile: *Students interested in theoretical and/or experimental electron quantum transport. Knowledge of quantum mechanics basics is required. Familiarity with MATLAB is desirable, though not strictly necessary.*