

Simulation of scanned probe spectroscopy: a challenging numerical problem

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Scanned probe spectroscopy is an interesting technique developed a few years ago [1,2] for the direct investigation of the flow of electrons and of the position of impurities in nanoscale devices based on a 2-dimensional electron gas. Initial applications [1,2] were to the electron gas obtained by modulation doping in a GaAs/AlGaAs heterostructure and, more recently, to that in a graphene sheet [3]. The basic concept of scanned probe spectroscopy consists in measuring the effect on the device conductance of the potential perturbation due to a negatively biased probe that is scanned over the region of interest of the device. By creating a map of the conductance values in correspondence with the probe positions, interesting information about current paths and impurity scattering can be obtained.

We have been interested in the numerical simulations of these experiments, in order to develop a tool providing a better understanding of what is actually measured in such experiments and a reliable estimate of the achievable resolution. Our initial work was focused on GaAs/AlGaAs heterostructures and, in the last year, we got interested in the simulation of scanned probe spectroscopy experiments performed on graphene flakes [3].

Simulation of this type of experiments requires indeed a significant computational effort, because in principle the conductance across the device has to be re-computed for each probe position. The conductance can be evaluated, via the Landauer-Buettiker formula, from the knowledge of the transmission through the device for a range of energies around the Fermi level. Transmission can be obtained, for example, by means of the recursive Green's function technique or the recursive scattering matrix technique. All of these methods include a first step in which the device is subdivided into slices, within each of which the potential is assumed to be longitudinally constant. Calculation of the transmission is in itself a computationally intensive task, if, at least in some regions, a large number of transverse modes are propagating; then this has to be repeated for a number of times corresponding to the possible positions of the scanning probe. Without some form of optimization, such a calculation would definitely be unfeasible. We have looked into several forms of optimization, starting from preventing the repeated calculation of the transverse wave functions of the sections: the transverse Schrodinger equation is solved again, at each step in the probe position, only for the slices which are directly affected by the probe potential. Furthermore, one could compute the Green's function matrix from each end of the device to any of the intermediate slices (in the absence of the probe), keep this information in memory, and reuse most of it at each scanning step (thereby computing from scratch only the Green's function matrices of the region whose potential is altered by the probe). There is clearly a trade-off in terms of memory occupancy vs. speed, because if we want to keep all of this information, quite significant an amount of memory will be needed. With such an approach we can obtain plots of the results of scanned probe spectroscopy of quantum point contacts (Fig. 1) or of mesoscopic cavities (Fig. 2) with a computational effort of the order of a CPU-day.

Further improvements could be achieved by treating the potential of the probe as a perturbation and recomputing the overall Green's function matrix via the Dyson equation. This has been done with success in Ref. [4], where the effect of the probe was assumed to be localized in a single grid-point. In principle, this approach can be extended to the case of a probe creating a generic perturbation of the

potential at the 2DEG level (usually assumed to be a Lorentzian), but the speedup is reduced and, depending on the size of the area affected by the potential perturbation, may not be convenient.

We are currently working on the implementation of scanned probe spectroscopy simulations of graphene flakes: such simulations pose a very challenging computational problem, since experiments are performed on flakes with a width of the order of 1 micron, which makes approaches based on the atomistic methods usually applied to graphene (such as tight-binding) unfeasible. Therefore we have chosen a continuum approach consisting in the solution of the Dirac equation in each transverse section (which corresponds to the equation for the envelope functions in the vicinity of the band degeneration points). The numerical solution of such an equation is, however, a very challenging problem in itself, due to the difficulties in finding a proper, consistent discretization. By extending the solution to a domain that is twice the width of the original domain, the boundary conditions become more standard and an efficient algorithm for the numerical solution can be implemented.

References

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Figures

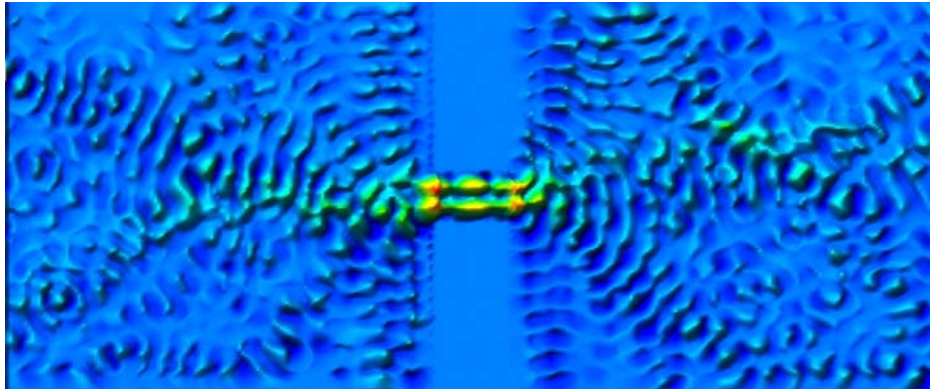


Fig. 1 Results for the scanned probe spectroscopy of a quantum point contact in the presence of a random potential due to dopants.

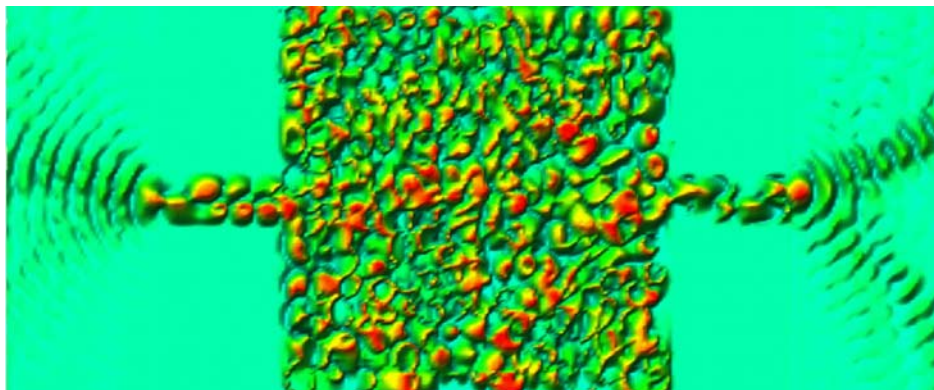


Fig. 2 Results for the scanned probe spectroscopy for a mesoscopic cavity, in the presence of the potential due to randomly located dopants.