Numerical simulation of the electron transport through graphene nanoribbons

Master thesis (research project, track MSCI)

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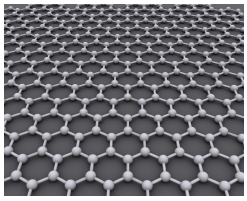
Keywords: PDEs, numerical simulations, eigenvalue computation, nanostructure modeling.

Context:



Graphene is a two dimensional material made of a honeycomb lattice of carbon atoms (see figure beside). Due to its extraordinary properties (in particular, its remarkable electronic properties [1]), it becomes a promising material for various applications (subject to the Nobel prize in 2010). Physical phenomena generated in graphene devices are extremly complex. In order to predict their behaviors, an important experimental test battery is necessary. In parallel, modeling and numerical simulations can play a significant role in the performance optimization of such devices.

Internship description:

The transport of electrons in graphene has been the subject of intensive recent studies in both mathematicians and physicists communities. In recent mathematical works (see e.g. [2]), spectral properties of the two dimensional Schrödinger operator $H = -\Delta + V_{per}$ (where V_{per} is a periodic potential having the symmetry of a honeycomb lattice) have been studied, in order to characterize the energy bands of an infinite graphene sheet.

The goal of this internship proposal is to study the transport of electrons through graphene nanoribbons GNRs. These structures are thin strips of graphene in which electrons are confined along a given longitudinal direction. Since the edges of GNRs break the lattice symmetries, the electronic states seem to be strongly dependent on their shape and on the boundary conditions taken along them. The two main objectives will be:
- to compute, using an appropriate numerical method, the energy bands of GNRs with different edges and to compare the obtained results with those found in the physics literature.
- to examine, using spectral analysis techniques, how the energy band properties (in particular the existence of conical singularities called Dirac points) depend on the choice of the boundary conditions and the nanoribbon geometry.

Prerequisites: Basic knowledge in PDEs (variational formulation of elliptic problems, Lax-Milgram theorem,...) and numerical analysis are required, as well as good programming skills. An additional interest in mathematical modeling of physical phenomena will be a plus.

[1] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim. The electronic properties of graphene. *Rev. Mod. Phys.*, 81:109–162, 2009.

[2] C. L. Fefferman and M. I. Weinstein. Honeycomb lattice potentials and Dirac points. *J. Amer. Math. Soc.*, 25:1169–1220, 2012.