Numerical simulation of the electron transport through graphene nanoribbons

Master thesis (research project, track MSCI)

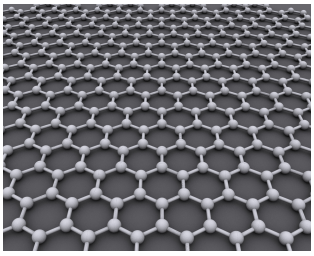
Advisors: Clément Jourdana (UGA) & Faouzi Triki (UGA), team EDP, LJK.
contact: clement.jourdana@imag.fr, +33 (0)4 57 42 17 47 ; triki@imag.fr, +33 (0)4 57 42 17 86

Location: Laboratoire Jean Kuntzmann
IMAG Building, 700 avenue centrale
38401 Saint Martin d'Hères

Keywords: numerical simulations, spectral analysis, electronic transport, nanostructure modeling.

Context:

Graphene is a two dimensional material made of a honeycomb lattice of carbon atoms. Due to its extraordinary properties, it becomes a promising material for various applications. In particular, it is 100 times stronger than the strongest steel and it exhibits a unique electronic band structure that allows an efficient conduction of electrons [1]. In this proposal, we are interested in the mathematical modeling of the electron transport through graphene nanostructures.



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]), the 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 nanorribons 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 main objective is to compute, using an appropriate numerical method, the energy bands of GNRs with given boundary conditions, and to compare the obtained results with those found in the physics literature.

Prerequisites:

Basic knowledge of partial differential equations and numerical methods are required. An additional interest in mathematical modeling of new 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.