APS March meeting 2016 tutorial
"Introduction to computational quantum nanoelectronics"

Handout

Sunday, 13 March 2016, 1:30 pm – 5:30 pm

Christoph Groth (CEA Grenoble, France)
Anton Akhmerov (TU Delft, The Netherlands)
Michael Wimmer (TU Delft, The Netherlands)
Xavier Waintal (CEA Grenoble, France)

Important note

This tutorial includes hands-on numerical programming exercises. To fully participate, please bring a portable computer that can operate on battery for four hours [1]. No software setup is required since we provide a web-based computational environment. Participants who would like to run the software directly on their own machines are welcome to do so: see Section 4.

Course materials are made available online at http://kwant-project.org/mm16/.

1 Overview

Quantum nanoelectronics deals with the physics of small (< 1 μm) and/or cold (down to ∼ 10 mK) objects connected to the macroscopic world through electrodes or gates. A central question at the core of this field is how quantum effects can be observed and manipulated through the macroscopic measuring apparatus.

In this tutorial, we will give a pedagogical introduction to the field. We will begin with an introduction to the main theoretical concepts and a review of some seminal experiments. The central part of the tutorial will be devoted to practical training on numerical calculations: we will demonstrate how researchers can simply setup their own models and perform their own calculations. These calculations can be used for theoretical predictions, to explain experimental data or even to assist the conception of device design.

[1] We do not know how many power outlets are available in the lecture room. Please try to bring a battery that supports (mostly idle) computer operation for the duration of the tutorial. If you think that you will have to recharge, please bring a multi-outlet extension cord with you.

2 Schedule

- Introduction (1 hour)
  - Theory refresher
  - Technical setup
  - Python refresher
- Basic numerical quantum transport (1 hour 15 minutes)
  - Discretizing continuum Hamiltonians into tight-binding, energy levels in a quantum dot
  - Translationally invariant systems and band structures
  - Scattering problem, leads, the S-matrix, "MOSFET transistor" toy model
  - Aharonov-Bohm effect
- break (15 minutes)
- Advanced numerical quantum transport (1 hour 30 minutes)
  - Quantum point contact
  - Quantum Hall effect and disorder
  - Graphene
  - Topological systems
  - Spintronics: giant magnetoresistance

3 Preparation

3.1 Theoretical introduction handout

Slides for the "Theory refresher" part of the lecture are distributed along with this document and can be downloaded at http://kwant-project.org/mm16/. For a more substantial introduction, we recommend a basic book on quantum nanoelectronics such as "Electronic transport in mesoscopic systems" by Supriyo Datta.

3.2 The Python programming language

No particular background in programming is needed, but we assume some programming experience. The numerical part of the lecture uses the Python programming language (version 3). Participants who are not yet familiar with Python may find the following useful:

- A web-based Python session can be started without any registration at http://python.org/: click on the prominent yellow button that is labeled with ">_".

- One may also directly start to use Python within a Jupyter notebook, see Section 3.4.
- https://python.org/about/gettingstarted/
- A Python tutorial geared towards scientists: http://software-carpentry.org/lessons/

3.3 Kwant

In the numerical part of the tutorial the Kwant Python package is used heavily. No prior knowledge of Kwant is required to participate, but interested participants may find the following useful:

- Kwant website: http://kwant-project.org/
- Kwant paper: http://downloads.kwant-project.org/doc/kwant-paper.pdf
- Kwant tutorial: http://kwant-project.org/doc/1/tutorial/

3.4 Jupyter notebooks

Jupyter (http://jupyter.org/) allows to create interactive documents that mix program code with the associated output, as well as additional text, mathematical formulas, images, etc. All the exercises of this tutorial are based on Jupyter notebooks that will be made available during the course.

An example live Jupyter notebook that demonstrates Kwant can be tried out online by browsing http://mybinder.org/repo/kwant-project/billiard/billiard.ipynb. This example is taken from the Kwant paper mentioned above. Use the "Help" menu to learn how to use the notebook. A new notebook can be opened from the "File" menu.

Attention: an online session will be deleted after one hour of idle time. To save a notebook, use "Download as" in the "File" menu. Uploading a previously downloaded ipynb file is possible in the notebook list (click on the Jupyter logo and then on "Upload").

Persistent online notebooks are available at http://cloud.sagemath.com/.

4 Software setup

While this tutorial can be followed without installing any software locally, all the involved software (Python, Jupyter and Kwant) can be run natively on all common operating systems. Doing so is recommended for serious use since it provides superior performance and availability. Participants who are motivated to install the software stack before the tutorial may find the following pointers useful.

- Installing Python and Kwant: http://kwant-project.org/install
- Installing Jupyter: http://jupyter.org/