

Recent progress in the simulation of time-resolved quantum nanoelectronics

B. Gaury, J. Weston, C. Groth and X. Waintal
Univ. Grenoble Alpes, INAC-SPSMS, F-38000 Grenoble, France
CEA, INAC-SPSMS, F-38000 Grenoble, France
e-mail: xavier.waintal@cea.fr

INTRODUCTION

Finite frequency quantum transport is a bit like particle physics; accessing higher frequencies in experiments unlocks new physics. Keeping in mind that 1 Kelvin corresponds roughly to 20 GHz ($h\nu = k_B T$), one finds that the recent technical progress made in putting RF lines (~ 10 GHz) in dilution fridges (~ 10 mK) opens the way for time-resolved coherent transport ($h\nu \gg k_B T$).

Perhaps the simplest time-resolved experiment one can do with a coherent conductor is to apply a voltage pulse $V(t)$ and monitor the current $I(t)$. A total of $\bar{n} = (e/h) \int dt V(t)$ electrons are sent through the device and new physics is expected in the quantum regime, i.e. when $\bar{n} \approx 1$. This regime has been recently observed by Glattli and colleagues [1].

This short lecture will consist of three parts.

I. DYNAMICAL MANIPULATION OF INTERFERENCE PATTERN

First, I will discuss a few intriguing physical effects which highlight how time resolved transport in the quantum regime can be fundamentally different from its DC counterpart. My chief example will be a simple electronic interferometer such as a Mach-Zehnder or a Fabry-Perot cavity. I will show that voltage pulses can be used to dynamically control the interference pattern of these interferometers [2]. This effect can give rise to DC currents that, counterintuitively, oscillate with \bar{n} .

II. FORMALISM

Simple concepts can often be understood at the analytical level, yet analytical approaches are often limited and/or time consuming. In order to treat problems further numerical calculations can be a

valuable asset. In the second part, I will review the mathematical formalism of quantum transport starting from the non-equilibrium Green function (NEGF) approach. NEGF provides a compact theory for time-resolved quantum transport but solving the NEGF equations is computationally prohibitive. Despite several attempts, it is difficult to go beyond systems of 10 – 100 degrees of freedom using NEGF alone. A competing approach based on Scattering wave functions is much more promising. A third approach where one does not partition the system into a central region connected to electrodes is also very appealing. These three approaches are in fact totally equivalent. I will show how one can construct a "source-well" wavefunction algorithm whose computing time is linear with both the size of the system and the physical time that is simulated [3]. Currently, simulations of systems with 100000 degrees of freedom have been demonstrated using this technique.

III. NUMERICAL ASPECTS

In the last part, I will discuss some practical aspects implementing this formalism. I will introduce the numerical code Kwant [4] and its time dependent generalization T-Kwant. Kwant implements the concept of a Hamiltonian in the Python programming language. The traditional "input files" are replaced by small programs that look very similar to what a scientist would write on the blackboard. 10 to 20 lines are usually enough to simulate a graphene flake, a topological superconductor with Majorana fermions or a quantum spin Hall semiconducting heterostructure. I will argue that in the same way that efficient algorithms save computing time, modern programming approaches save a lot of time for the scientist.

REFERENCES

- [1] J. Dubois, T. Jullien, F. Portier, P. Roche, A. Cavanna, Y. Jin, W. Wegscheider, P. Roulleau and D. C. Glattli, *Minimal-excitation states for electron quantum optics using levitons*, Nature **502**, 659 (2013).
- [2] B. Gaury and X. Waintal, *Dynamical control of interference using voltage pulses in the quantum regime*, Nat. Commun. 5:3844 doi: 10.1038/ncomms4844 (2014). ArXiv1401.5280
- [3] B. Gaury, J. Weston, M. Santin, M. Houzet, C. Groth and X. Waintal, *Numerical simulations of time-resolved quantum electronics*, Physics Reports **534**, 1 (2014).
- [4] C. W. Groth, M. Wimmer, A. R. Akhmerov and X. Waintal, *Kwant: a software package for quantum transport*, ArXiv1309.2926, to appear in New J. Phys. (2014). Kwant web site: <http://kwant-project.org>