Recent progress in the simulation of time-resolved quantum nanoelectronics

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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 ($\hbar \nu \approx k_B T$), one finds that the recent technical progress made in putting RF lines ($\sim 10$ GHz) in dilution fridges ($\sim 10$ mK) opens the way for time-resolved coherent transport ($\hbar \nu \gg k_B T$).

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 $\bar{n} = (e/\hbar) \int dt V(t)$ 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 semi-conducting 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


