Joule heating in atomic wires

Background

On a cold winter's morning we go to the kitchen, put the kettle on and soon after we can enjoy a comforting hot drink. This miracle is due to one of the fundamental processes in electrical conductors: the electron-phonon interaction. Phonons are the thermal vibrations of the atoms. The electrons that carry the current disturb the atomic nuclei, they start to swing more energetically, and the result is what we know as Joule heating.

Now imagine this phenomenon in the thinnest possible wires in nature: chains of single atoms. These systems have been experimentally possible for about 30 years using techniques one of which – the Scanning Tunnelling Microscope – won the Nobel Prize. This is a horrendously hard problem theoretically. Why? Because electrons are strictly quantum particles and a consistent theory of the energy exchange requires the nuclei to be treated quantum mechanically too, while taking account of the interactions between the two. This turns it into a quantum many-body problem, and these are the hardest class of problems in condensed matter physics.

The project

There is a host of different techniques that have been proposed for this problem, notably Non-Equilibrium Green's Functions and Correlated Electron-Ion Dynamics (co-developed between Belfast and London), including some very recent work on combining the electron-phonon aspect with electron-electron interactions. However they are computationally extremely demanding and – more importantly – the atomic motion can only be considered at the level of quantum correlation functions which makes it impossible to visualise the dynamics of the individual atoms in a classical framework.

In this project we will implement a recent idea, developed by researchers in Belfast and Denmark, that maps the quantum electron-phonon problem into an *effective* semi-classical problem in which the nuclear motion is classical but there are special additional forces due to the electrons that subsume all the quantum mechanics. One has to solve the quantum Liouville equation for the electronic density matrix concurrently with the effective classical equations of motion for the nuclei, except that the Liouville equation also acquires special terms that take account of the correlated interactions with the phonons.

This idea has been tested on simple model systems but has never been fully developed or implemented. Doing so is the aim of this work.

Requirements and benefits

A background in quantum mechanics, combined with a pronounced ability for pen and paper theory and good computational skills. This is a tough but exciting project that will result in a set of skills at the cutting edge of condensed matter theory. We have long-standing links with theorists and experimentalists in Denmark and the Netherlands, as well as here at Queen's, which will make this a highly collaborative project. Above all, it will form an integral part of an ongoing collaboration with Trinity College Dublin on this very problem.

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