Eric Ceccarelli

Moving on boxes

The conduction of electricity is a crucial feature of materials. However the movement of electrons is challenging to predict due to the interactions between them. Further complicating the problem, the electrons are also affected by the movement of the atoms. This thesis investigates the effect the atomic vibrations in a molecular junction have on the electric current flowing across it.

Electricity is a vital resource of our everyday life. It is safe to say that without it the world would not look the way it does today and that our society depends on it. Unfortunately, a great part of the electric power created in power plants is lost during transport and distribution. A solution to this problem could be by utilizing superconductors. A superconductor is a material that transports electricity with little to no loss. Superconductors are a topic of current research since they currently only perform at low temperatures. The invention of a room temperature superconductor has the potential to spring many new technologies.

The conduction in a microscopic solid material is challenging to study since molecules, which are clusters of atoms, tend to vibrate. We can think of the molecules in a molecular solid as boxes that are aligned in a straight line. Each box is connected to the closest one by a spring. We can then imagine a small toy car that is placed on top of them and can only move from one box to the next. Its movement causes motion to the boxes. If a box is moved from its initial position, because of the car, it will stretch the spring by which it is attached to the adjacent ones. When released it will create an oscillation in the line since every box is connected. The movement of the toy car is then in turn affected by the movement of the boxes. Then imagine multiple cars moving on the boxes together in a cluster. Each car affects the movement of the others since they can touch each other. These interactions become problematic for a large number of cars. In our analogy the molecules, which are connected by a force, are represented by the boxes connected by the springs. The vibration of the molecules is represented by the movement of the boxes and the electrons are represented by the toy cars that, just like in the analogy, are affected by each others movement and that of the molecules.

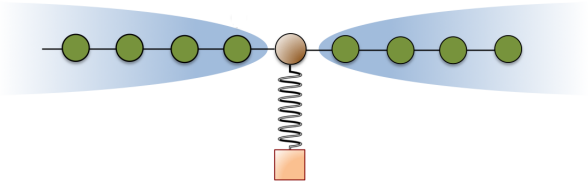

Figure 1: *A simple schematic of the system.*

In this thesis a simulation of a molecular junction with electrons flowing across it is performed. The atoms composing the molecule are allowed to vibrate. In an oversimplified version of this problem we can imagine the molecular junction as to be attached to a spring in the vertical direction as shown in figure 1. The interaction between electrons is accounted for by introducing an effective interaction amongst them. The aim of this thesis is to analyze how the simultaneous effect of the electronic interactions and the molecular vibration affect the current of electrons that flows through a molecular junction.

Supervisor: **Claudio Verdozzi**
Thesis submitted for the degree of: bachelor 15hp
Department of physics