Contents

Chapter 1

Basic concepts of the research field

Abstract

In this chapter, the basic concepts of electrical conductance in atomic and molecular junctions are discussed. Depending on the size of the contact, different regimes are expected. Electron tunneling and conductance quantization is explained together with characteristic measurements. Finally, we discuss how atomic or molecular levels and also vibrations can be observed in the measurements.

1.1 Conductance at the atomic scale

1.1.1 Semiclassical description

When considering a metallic wire of macroscopic dimensions, the electrical resistance of such a wire is simply given by Ohm's law. This relation states that the current through a wire (I), is proportional to the voltage over the wire (V), with 1/R as the proportionality constant (R is the resistance):

$$I = \frac{V}{R} \tag{1.1}$$

This relation was first found by Henry Cavendish in 1871, but named after Georg Ohm, who was the first to publish his experiments [1]. The existence of resistance is an important issue in daily life. For example, the resistance of a wire in a light bulb leads to lighting, or is used in heating systems, as described by Joule heating (given by I^2R). Interestingly, although these systems are of macroscopic size, the origin of resistance lies at the nanometer scale. Finally, it is all described by how easy electrons can move through a metallic conductor. This can be explained by the following: Let us assume a metallic wire, at zero temperature, where the atoms are perfectly ordered in a lattice. When a voltage is applied over the wire, the electrons will be accelerated from one side of the wire to the other. In this hypothetical case, the electrons will not be hindered, leading to an infinite current through the wire. However, it is not possible to create such a wire. A metal will always have impurities or imperfections of the lattice. Hence, electrons can only travel a limited length, before they are scattered to these irregularities in the metal. This scattering always gives a nonzero resistance, leading to the relation described above.

We note here that scattering can actually occur in two ways: When energy is exchanged during the scattering process, one talks about inelastic scattering. This happens when electrons scatter with other electrons, or when electrons excite lattice vibrations (phonons). This process is responsible for macroscopic processes like heating. Besides inelastic scattering, elastic scatter events take place. In general, this refers to scattering with ions in the lattice. Since these ions have a much larger mass then the electron, no energy is transferred and the phase of the electron is conserved. We briefly state here that this process can result in conductance fluctuations; according to quantum mechanics, a moving electron can also be described as a wave. Due to elastic scattering, an electron can follow the same path for multiple times, without losing its phase information. Hence, this can result in destructive interference, which can have a large influence on the conductance properties of mesoscopic systems. Finally, we note that both quantities are described by length scales; the mean length the electron travels before scattered elastically (inelastically), is called the elastic (inelastic) scattering length.

Bibliography

[1] T. Jain, F. Westerlund, E. Johnson, K. Moth-Poulsen, and T. Bjrnholm, "Self-assembled nanogaps via seed-mediated growth of end-to-end linked gold nanorods," *ACS Nano*, vol. 3, pp. 828–834, 2009.