Quantization of conductance in nanowires

PHYS-E0411 Advanced Physics Laboratory

Laboratory instructions

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1 Introduction

In electronics we describe the flow of current through an Ohmic conductor of resistance R by writing the Ohm's law $I = V/R$. Here V is the voltage applied across the resistor and I is the current flowing through it. We do not worry about the microscopic description of the flow of electrons in the conductor. As an example of an Ohmic conductor we consider a wire of length L, transversal area S and material-dependent resistivity ρ. The resistance of the wire is $R = \rho L/S$. We see that the conductance $G = R^{-1}$ depends on the material and should approach zero smoothly (continuously) as the area is decreased. However, experiments show that in sufficiently narrow wires the conductance is material-independent and decreases in quantized steps as the area is reduced. The step size $G_0 = 2e^2/h \simeq 7.7 \cdot 10^{-5} \ \Omega^{-1}$ is called the quantum of conductance.

It has been shown [1] that nanowires can be obtained by placing in contact two metals of any size and then separating them. At the last stages of breakage of the macroscopic contact between the two metals, the dimensions of the contact are in the nanometer scale and nanowires are formed. This can take place at ambient conditions without any sophisticated equipment! This laboratory work gives you a chance to experimentally observe quantization steps in conductance by measuring conductance of a loose electrical contact formed between two thin gold wires ($25\mu m$ in diameter each).

The gold wires are soldered to thicker wires and the thick wires are soldered to BNC connectors. The BNC connectors are used to connect the wires
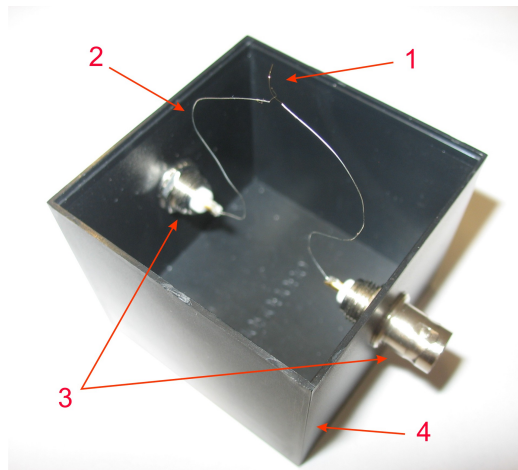

Figure 1: Wires holder: 1 - thin gold wires, 2 - thicker wires, 3 - BNC connectors, 4 - plastic box.

to the measurement electronics. The connectors are attached to the opposite walls of a plastic box (see Fig.1), which plays the role of a wires holder. By tapping the table top on which the wires holder sits or by shaking the holder itself, you can easily trigger vibrations of the thin wires. During this process the wires move back and forth to each other and the loose electrical contact breaks down and forms again many times. Nanowires form every time when the contact is breaking down (at the very last instants of its existence). We probe the conductance of this loose contact by applying a constant voltage V_0 over the wires and measuring the current flowing through the contact. The measured current $I = GV_0$ is directly proportional to the conductance of the contact G.

Let us first consider the theoretical justification of conductance quantization and then describe the experimental setup and settings allowing one to observe the steps in conductance.

2 Theoretical background of conductance quantization

To understand the origin of the effect of conductance quantization we can use some results of quantum transport theory in the so-called Landauer-Büttiker approach. Within this approach electrons flow ballistically through the wire. This assumption is valid when the size of the wire is small. Let us consider a simple quantum mechanical problem in which this wire is modelled as a waveguide with finite width and thickness (x and y directions) and an infinite length in the z direction. The time-independent Schrödinger equation for the electrons in the wire is

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + U(x,y,z) \right] \psi(x,y,z) = E\psi(x,y,z). \tag{1}$$

We simplify the problem by assuming that the potential U is independent of the coordinate z inside the nanowire. This allows us to use the method of variables separation to search for a solution in the form

$$\psi(x,y,z) = \chi(x,y)e^{ik_z z}, \tag{2}$$

which yields

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + U(x,y) \right] \chi(x,y) = \left(E - \frac{\hbar^2 k_z^2}{2m} \right) \chi(x,y). \tag{3}$$

Next, we should specify the lateral boundary conditions. Since usually work potential of a few eV is required to extract electrons out of the metal, we can use the rectangular box model potential - the potential is zero inside the box and it abruptly rises to infinity at the box edges so that the electrons are confined laterally and their wavefunction vanishes at the edges,

$$\chi(0, y) = \chi(L_x, y) = \chi(x, 0) = \chi(x, L_y) = 0, \tag{4}$$

with L_x and L_y the transversal dimensions of the wire. One can easily check that the solution is

$$\chi^{(n_x, n_y)}(x, y) = A_n \sin(k_{n_x} x) \sin(k_{n_y} y), \tag{5}$$

with $k_{n_x} = \frac{\pi n_x}{L_x}$, and $k_{n_y} = \frac{\pi n_y}{L_y}$, so

$$\epsilon^{(n_x, n_y)} = E - \frac{\hbar^2 k_z^2}{2m} = \frac{\hbar^2}{2m}(k_{n_x}^2 + k_{n_y}^2) = \frac{\hbar^2 \pi^2}{2m}\left(\left(\frac{n_x}{L_x}\right)^2 + \left(\frac{n_y}{L_y}\right)^2\right). \tag{6}$$

From here we get the longitudinal wavevectors in the form

$$k_z^{(n_x, n_y)} = \pm \sqrt{\frac{2m}{\hbar^2}\left(E - \frac{\hbar^2 \pi^2}{2m}\left(\left(\frac{n_x}{L_x}\right)^2 + \left(\frac{n_y}{L_y}\right)^2\right)\right)}. \tag{7}$$

The group velocity of the electrons in the z direction is by definition

$$v_z^{(n_x, n_y)} = \frac{d\omega}{dk_z^{(n_x, n_y)}} = \frac{1}{\hbar}\frac{dE}{dk_z^{(n_x, n_y)}} = \frac{\hbar k_z^{(n_x, n_y)}}{m}. \tag{8}$$

For a propagating wave $k_z^{n_x, n_y}$ is a real number. Thus, only the states for which the expression under the root in the equation (7) is positive can carry current. In other words, the energy $\epsilon^{(n_x, n_y)}$ related to the transverse mode $\chi^{(n_x, n_y)}$ should be smaller than the energy E. If we assume that the total energy of the electron is $E = eV_0$, where V_0 is the voltage applied over the contact, we find that only a finite number of pairs (n_x, n_y) satisfy the condition. This number of pairs is the number of longitudinal modes which can carry current.

The second result of the Landauer-Büttiker formalism relevant here is that the current per longitudinal mode through the wire with the voltage V_0 applied across it reads

$$I = \frac{2e^2}{h}V_0. \tag{9}$$

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This gives us the conductance per longitudinal mode $G_0 = I/V_0 = 2e^2/h$. If there are N conducting channels available then the conductance will be equal to $G = 2e^2 N/h$. Disappearance of one conductance channel leads to the drop in the conductance by G_0, which explains the fact that the conductance of a nanowire reduces in steps.

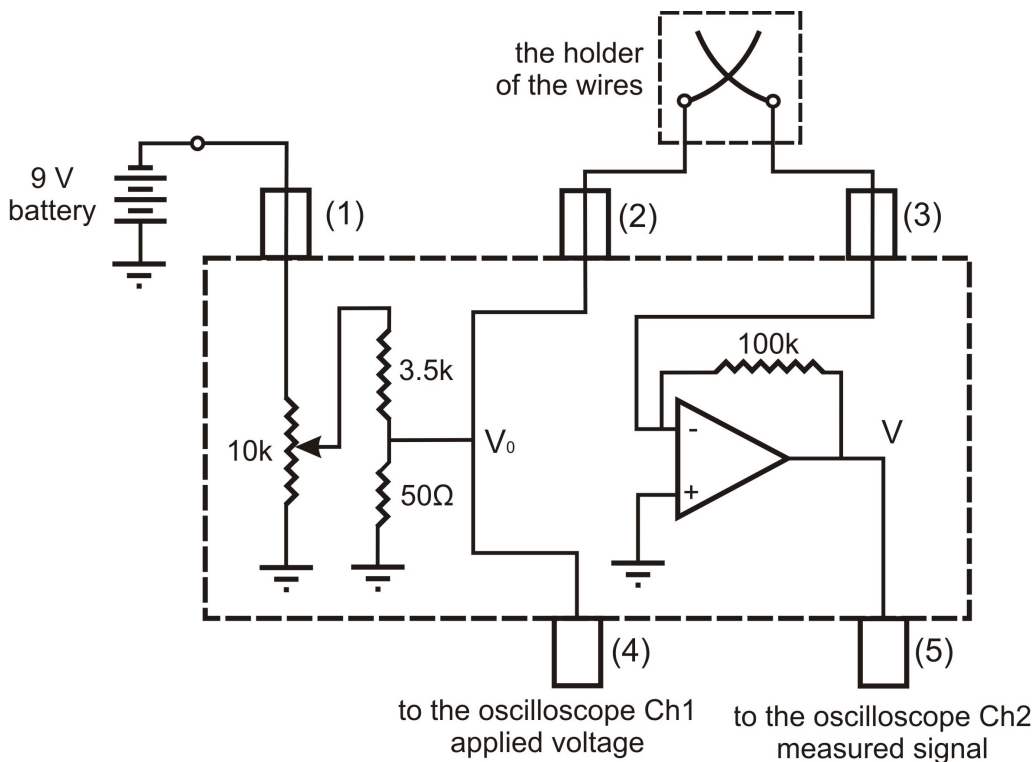# 3 Experimental setup and measurements

Figure 2: Diagram of the box with the electronics.

The experimental setup consists of three main parts: metal box, which comprises all the electrical components needed for the experiment, holder of the wires and an oscilloscope. The diagram of the setup is presented in Fig. 2. The metal box has a circuit board inside with a tunable voltage source and a current to voltage converter assembled on it. The voltage source is powered from a 9V battery, which is connected to the BNC connector (1) of the box. This source can give the output voltage in the range from 0 to roughly 120 mV. You can monitor this voltage by connecting the channel 1 of the oscilloscope to the connector (4) of the metal box. The output voltage from

the voltage source is applied to one of the wires of the nanocontact from the connector (2) of the box. The second wire of the nanocontact is connected to the connector (3) of the box and then further to the inverting virtual-ground input of the operational amplifier of the current to voltage (I - V) converter (see Fig.2). The output of the converter is fed to the connector (5) of the box and can be measured by channel 2 of the oscilloscope. As a result the voltage displayed on the channel 2 of the oscilloscope is proportional to the current flowing through the contact.

The voltage applied to the wires should be in the range of few tens of mV (we recommend you to use 20 mV voltage). Higher voltages will cause substantial heating effects whereas much smaller voltages lead to problems with the signal-to-noise ratio.

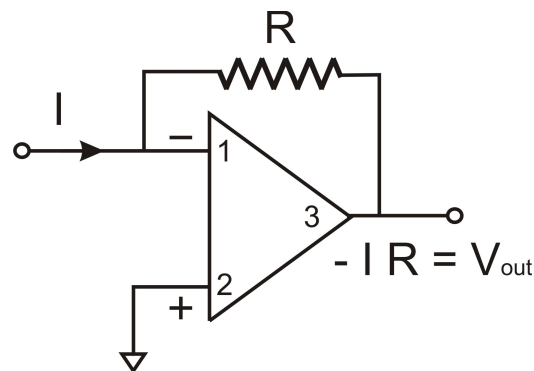**Current to voltage converter**

Figure 3: Scheme of a current to voltage converter.

To determine conductance of an element, one needs to know the current going through this element and the voltage drop across it. Current and voltage should be measured independently, but in many experiments it is more convenient and easy to measure only voltages. Therefore, it is good to know how one can convert a current signal to a voltage signal. Such conversion can be implemented with the use of a simple circuit based on an operational amplifier and is called current to voltage (I-V) converter (see Fig. 3). The operational amplifier has two signal inputs (1 and 2) and one output 3. The output 3 is connected via a resistor R to the input 1 of the amplifier, forming a feedback loop. The input 2 is connected to the ground. We feed the current, which we want to measure, to the input 1.

There are two basic rules concerning an ideal operational amplifier connected with a feedback loop. The first rule is that the voltage difference

between the inputs 1 and 2 is always zero. Since input 2 is connected to ground, input 1 must be in ground potential as well. This is called virtual grounding. The second rule is that the impedance between the two inputs is infinite, so zero current flows from input 1 to input 2. Thus, all the current we feed to input 1 goes through the feedback resistor R. The voltage of the amplifier output is then $V_{out} = -I_{in}R$. From here we can see that once we know the resistance of the feedback resistor we can determine the current I_{in} from the measured voltage V_{out}. The I-V conversion coefficient of the converter is $k = 1/R = -I_{in}/V_{out}$.

Preparation of the setup

Further you can find instructions how to collect the data required for the observation of steps in conductance. We start the measurements by determining the conversion coefficient of the I-V converter.

- Check that the following settings are applied on the oscilloscope:
  For the Channel 1 and Channel 2:
  - Coupling $\rightarrow$ DC
  - BW limit $\rightarrow$ Off
  - Probe $\rightarrow$ 1xVoltage
  - Input $\rightarrow$ 1MΩ
  - Invert $\rightarrow$ Off
  - Volts/Div $\rightarrow$ Coarse
  - Unit $\rightarrow$ V
  - 20 mV/div (for Channel 1) and 500 mV/div (for Channel 2)
  For the trigger:
  - Type $\rightarrow$ Edge
  - Source $\rightarrow$ Ch2
  - Slope $\rightarrow$ Falling
  - Mode $\rightarrow$ Auto
  - Coupling $\rightarrow$ DC

- Connect one of the 9V batteries to the connector (1) of the metal box and the other two batteries to the wires coming out of the hole in the metal box.

- Using BNC cables connect the outputs (4) and (5) of the metal box with the inputs of the Channel 1 and the Channel 2 of the oscilloscope, respectively.

- Measure the resistance of the resistor R_0 (provided by the assistant) with a multimeter and make a note of the value. Make sure the applied voltage is

set to 0 by turning the knob on the metal box. Connect the resistor between the connectors (2) and (3) of the metal box.

• By turning the knob on the top of the metal box, set the voltage V_0 over the resistor to ~ 20 mV. Read the voltage from the oscilloscope (Channel 1) and make a note of the value.

• Measure the output voltage V_{out} of the current to voltage converter (Channel 2) and make a note of the value. You will need the values R_0, V_0 and V_{out} to determine the conversion coefficient k of the I-V converter.

• Estimate the uncertainty in V_{in} and V_{out}. For this increase the sensitivity of the oscilloscope until noise is clearly visible. The position of the trace on the oscilloscope may have to be altered as you do this.

• Disconnect the resistor R_0 and connect the wires holder to the connectors (2) and (3) of the metal box instead. Adjust the voltage applied to the wires to 20 mV (channel 1).

• Switch the trigger mode of the oscilloscope to the Normal Mode. Set the time scale to 100 μs /div and the trigger level higher than 3 divisions.

• Insert the USB stick and check that the oscilloscope can read it. The USB stick might have to be formatted!

Data acquisition

The setup is now ready for the experiment and you can start the data acquisition. Shake the holder of the wires or hit it slightly to trigger the vibration of the wires. Sometimes the wires start to oscillate together so that the contact between them does not break. Other times the contact breaks too fast and it is not possible to detect steps in conductance. It usually takes many attempts to break the contact in proper way. It is important to have the gold wires clean, otherwise formation of nanowires will not be possible. Cleaning of the wires can be done by gently wiping them with a very soft tissue, napkin, or a cotton bud soaked with acetone. Too harsh cleaning procedure will break the wires, so be gentle.

It takes some patience and many repetitions to observe good voltage traces. You should see falling traces on the oscilloscope channel 2 with clearly visible steps on them. Such kind of a traces we call good ones. Try to repeat this many times and every time you get a good trace save it to a memory

stick. To do this you:

- Choose file type: CSV

- Press "Save"
    Give a filename (press OK and enter).

The data will be stored in a .CSV (comma separated values) file. Try to produce at least 15 good traces to have enough data for further processing.

Prerequisite Questions

1) In the classical description, how does the electrical conductance of a wire depend on the cross-sectional area of the wire? How does conductance depend on the applied voltage?

2) Does the classical picture hold for arbitrarily narrow wires? If not, how does the picture break down?

3) How does the conductance of a wire depend on the transversal dimensions of the wire in the quantum mechanical description? How does the conductance depend on the applied voltage?

4) What are the two basic rules of an operational amplifier?

5) How does an I - V converter based on an operational amplifier work?

Report

Include your answers to the above prerequisite questions in your report. In addition, address the following questions:

6) What is the value of the quantum of conductance G_0?

7) Calibrate the I-V converter: express the I-V conversion coefficient $k = 1/R$ in terms of R_0, V_0 and V_{out}, where R_0 is the resistance of the resistor used in the calibration of the setup, V_0 is the voltage applied over the resistor and V_{out} is the measured output voltage of the I-V converter. What is the value of k? Give an error estimate for the value of k.

8) Derive an expression to convert the measured voltage V_{out} to conductance G of the contact using the I-V conversion coefficient k and the applied voltage V_0. Give an error estimate for the value of G.

9) What is the mean free path of electrons in gold at room temperature? What is the size of wires for which the Landauer-Büttiker approach is valid?

10) Compare the thermal energy of electrons at room temperature with the work function of gold. Can you say something about the boundary conditions discussed in section 2 based on this?

11) Derive the energy levels of a particle in the infinitely deep 2D rectangular box potential

$$U(x,y) = \begin{cases} 0 \leq x \leq L_x, \ 0 \leq y \leq L_y, \\ +\infty, \ x \notin (0; L_x) \text{ or } y \notin (0; L_y). \end{cases}$$

Here L_x and L_y are the spatial dimensions of the potential box.

12) Based on the theory (sect. 2), derive an expression which gives an upper limit to the quantum numbers n_x and n_y. Using this expression, calculate the number of conductance channels, when $V_0 = 20$mV and $L_x = L_y = 10$ nm. What is the conductance of such a nanowire?

13) Choose the best voltage trace you got in your measurements. Convert the measured voltage to conductance G and normalize it to the units of quantum of conductance ($G_{\text{norm}} = G/G_0$). Plot the normalized conductance G_{norm} as a function of time. Matlab command *readmatrix()* can be used to read the .csv files. Describe in your own words how quantization of conductance is observed in the figure.

14) Use all the traces you have measured and plot a histogram of all the normalized conductance values. MatLab function *histogram()* may be helpful. Choose the number of bins (of equal width) in a way that best illustrates the data. Based on the theory (section 2), how would you expect the histogram to look like? Consider possible reasons why deviation from the ideal behaviour may be seen.

References

[1] J.L.Costa-Krämer, N.Garcia, P.Garcia-Mochales, P.A.Serena. *Nanowire formation in macroscopic metallic contacts: quantum mechanical conductance tapping a table top*, Surface Science **342** (1995), L1144-L1149.