Studies and Measurements of Electrical and Thermal Properties of Nanosystems

Waldemar Nawrocki
Faculty of Electronics and Telecommunications, Poznan University of Technology, Poznan, Poland
Email: nawrocki@et.put.poznan.pl

Yury M. Shukrinov
Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna, Russia
Email: shukrinv@theor.jinr.ru

Abstract—T In last 20 years considerable attention has been focused on investigations of both electrical and thermal properties (especially conductance) in nanosystems. The theoretical quantum unit of electrical conductance $G_0 = 2e^2/h = (12.9 \text{ kG})^2$ was predicted by Landauer [1] in his new theory of electrical conductance. The quantization of electric conductance depends neither on the kind of metal nor on temperature. The quantization of conductance in our experiment was evident, all characteristics showed the same quantization steps equal to $2e^2/h$. First theoretical analyses of thermal conductance in structures in the ballistic regime were made by P. Streda. Both electrical and thermal conductance of a nanostructure describe the same process: the electron transport. Beside observations of electrical conductance quantization in nanowires one can expect the thermal conductance quantization as well. Electron transport in a nanowire does two effects: an electrical current $I = G_0 \Delta V$, and a heat flux density $Q_0, Q_T = G_T \Delta T$, where $G_T$ – electrical conductance of a sample, $\Delta V$ – difference of electrical potentials, $G_T$ – thermal conductance of a sample, $\Delta T$ – temperature difference. $G_0 = \sigma A L k_B T$, $G_T = \lambda A/L$, where $\sigma$ is electrical conductivity, $\lambda$ is thermal conductivity, $L$ is length of a sample, $A$ area of a cross-section of a sample. Quantized thermal conductance in one-dimensional systems (e.g. nanowires) was predicted theoretically using the Landauer theory. In one-dimension systems conductive channels are formed. Each channel contributes to a total thermal conductance with the quantum of thermal conductance $G_{T0}$. Quantized thermal conductance and its quantum $G_{T0}$ was confirmed experimentally by Schwab. The quantum of thermal conductance $G_{T0}$ [W/K] = $(\frac{e^2 k_B T}{2\pi h})\Delta T$. Electron transport in the nanowire itself is ballistic, it means the transport without scattering of electrons and without energy dissipation. The energy dissipation takes part in terminals. Because of the energy dissipation the local temperature $T_{term}$ in terminals is higher than the temperature $T_{wire}$ of nanowires itself. A heat distribution in terminals of a nanostructure should be analyzed.

Index Terms—nanosystems, electrical conductance, thermal conductance, quantization, integrated circuits

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I. INTRODUCTION
The classical theory of electrical and thermal conductance, proposed by P. Drude in 1900, assumes a huge number of atoms and free electrons. However, number of atoms and free electrons in a nanostructure is not sufficiently large for a statistical description of their behavior. The electrical and thermal properties of nanostructures are described much better by the theory introduced by R. Landauer in 1989 [1]. Both the electrical conductance and the thermal conductance of a nanostructure are quantized. The theoretical quantum unit of electrical conductance $G_{T0} = 2e^2/h$ was predicted by Landauer [1]. In 1987 Gimzewski and Moller published results on measurements of the quantization of electrical conductance in metals at room temperature using a scanning tunneling microscope [2]. In 1988 two groups reported the discovery of the conductance quantization in controllable two-Dimensional Electron Gas (2DEG) in the GaAs constriction at the temperatures less than several kelvin [3], [4]. First theoretical analyses of thermal conductance in structures in the ballistic regime were made by Streda [5]. Quantization of thermal conductance and its quantum (unit) $G_{T0}$ was confirmed experimentally by Schwab [6]. The quantum of thermal conductance depends on two fundamental physical constants and on temperature: $G_{T0} = \frac{f(k_B, h, T)}{\Delta T}$.

II. ELECTRICAL AND THERMAL CONDUCTANCE OF NANOSYSTEMS
Let us consider conductor with diameter $W$ and the length $L$ (Fig. 1) connecting two wide terminals (referred as reservoirs of the electrons), where $L$ is shorter than the mean free path $\lambda$. The condition: $L < \lambda$ means that the electron transport along the conductor is ballistic. An important parameter of the nanosystem is the Fermi wavelength $\lambda_F = 2L/k_F$, where $k_F$ is the Fermi wave-vector. Metals such as copper or gold have a Fermi wavelength $\lambda_F = 0.5 \text{ nm}$, much shorter than the electron mean free path $\lambda$ (nm).

If the dimensions of the system are smaller than the electron mean free path, the scattering due to the presence
of impurities can be neglected, and, consequently, the electron transport can be regarded as ballistic. A metal wire with an external diameter \( W \) comparable with the Fermi wavelength \( \lambda_F \) and a length \( L \) shorter than can be treated as a one-Dimensional (1D) waveguide, with electrons regarded as waves, and quantum effects can be expected to occur. An object of a width comparable to the Fermi wavelength \( \lambda_F \) can be treated as a quasi-one-dimensional waveguide. Also in this case electrons are regarded as waves, and quantum effects can be expected to manifest their quantum nature.

Figure 1. Conductance quantization in a nanowire (conductor with the width \( W \) comparable with the length \( L \) shorter than can be treated as a one-Dimensional (1D) waveguide, with electrons regarded as waves, and quantum effects can be expected to occur. An object of a width comparable to the Fermi wavelength \( \lambda_F \) can be treated as a quasi-one-dimensional waveguide. Also in this case electrons are regarded as waves, and quantum effects can be expected to manifest their quantum nature.

If the conductor (nanowire) has the cross-section comparable with the Fermi wavelength \( \lambda_F \), the system can be considered as one-dimensional and quantum effects occur in the system. On the assumption that the electron reservoirs are infinitely large, the electrons are in thermodynamic equilibrium described by Fermi-Dirac statistics. When electrons enter the 1-D conductor, nonequilibrium states with negative and positive velocities appear. If a resultant current flows through the conductor, states with positive velocities have higher energy [1]. According to the Büttiker [8] model the Hamiltonian of the perfect conductor can be expressed as follows:

\[
H = \frac{1}{2m} \left( \hbar^2 k_x^2 + \hbar^2 k_y^2 \right) + V(x)
\]  

where \( y \) is the coordinate along the wire, \( x \) is the coordinate in the transverse direction, \( m^* \) is the effective mass, \( V(x) \) denotes the potential well of the width \( W \), \( k_x \) is the wavevector component along the \( y \) axis, and \( k_y \) is the wavevector component in the \( x \) direction. Because of the narrowness of the potential well \( V(x) \) the energy in the transverse propagation is quantized:

\[
E_{jL} = \frac{\hbar^2 k_x^2}{2m^*} = \frac{\hbar^2}{2m^*} \left( \frac{j\pi}{W} \right)^2
\]

The formula (2) holds if the potential energy tends to infinity at the boundary of the quantum well. For the Fermi level \( E_F = E_l \), there are \( N \sim 2W/L \) states \( E_{jL} \) below the Fermi level. Let us assume that the thermal energy \( k_B T \) is much lower than the energy gap between levels, and that the wide contacts have chemical potentials \( \mu_1 \) and \( \mu_2 \), with \( \mu_1 > \mu_2 \). Then, the current of electrons in the \( j \)-th state is:

\[
I_j = e v_j \left( \frac{dn}{dE} \right)_j \Delta \mu
\]

where \( v_j \) is the velocity along the \( y \) axis and \( (dn/dE)_j \) is the density of states at the Fermi level for the \( j \)-th state.

Hence, the current related to the \( j \)-th state, \( I_j = 2e^2 \Delta V \) (where the voltage difference \( V = \mu_2 - \mu_1 \), does not depend on \( j \). The total current is \( I = \sum_{j=1}^{N} I_j \). Consequently, the conductivity can be expressed as:

\[
G = \frac{2e^2}{h} N
\]

where \( N \) depends on the width of the wire (Fig. 1).

Measurements of electrical resistance (or conductance) of samples of a size close to (mesoscopic range) show that the Landauer theory describes the electrical conduction in such samples better than the Drude model. The conductance \( G \) of a single channel, with \( T_j = 1 \), is:

\[
G_e = \frac{2e^2}{h} \approx 77.2 \times 10^{-6} \text{ A/V} = (12.9 \text{ k} \Omega)^{-1}
\]

Measurements of electrical resistance (or conductance) of a sample of the atomic size show that the Landauer theory better describes real parameters of the sample. Both electrical \( G_E \) and thermal \( G_T \) conductance of a nanostructure describe the same process: electron transport in nanostructures. Therefore there are several analogues between the two physical quantities. Beside observations of the electrical conductance quantization in nanowires one can expect the thermal conductance quantization as well. Electron transport in a conductor demonstrates two effects: an electrical current \( I \) and a heat flux density \( Q_D \).

Electrical current: \( I = G_E \times \Delta V \)

Heat flux density: \( Q_D = G_T \times \Delta T \)

where \( G_E \) - electrical conductance of a sample, \( \Delta V \) - difference of electrical potentials, \( G_T \) - thermal conductance of a sample, \( \Delta T \) - temperature difference.

\[
G_E = \sigma \times A/L, \ G_T = \lambda \times A/L
\]

where \( \sigma \) is electrical conductivity, \( \lambda \) is thermal conductivity, \( L \) is length of a sample, \( A \) area of a cross-section of a sample.

Quantized thermal conductance in one-dimensional systems (e.g. nanowires) was predicted theoretically by Rego [7] and measured by Tanaka [8]. The thermal conductance is considered in a similar way like the
electrical conductance. In one-dimension systems are formed conductive channels. Each channel contributes to a total thermal conductance with the quantum of thermal conductance $G_{T0}$ as we mentioned above. Quantized thermal conductance and its quantum (unit) $G_{T0}$ was confirmed experimentally by Schwab [6]. The quantum of thermal conductance

$$G_{T0} [W/K] = (\pi^2 k_B^2 / 3h)T = 9.5 \times 10^{13} T \quad (6)$$

depends on the temperature (6), at $T = 300$ K, the value of $G_{T0} = 2.8 \times 10^{10} [W/K]$. This value is determined for the ideal ballistic transport (without scattering) in a nanowire, with the transmission coefficient of 100%. It means that in all practical cases the thermal conductance is below the limit given by formula (6).

Electron transport in the nanowire itself is ballistic, it means the transport without scattering of electrons and without energy dissipation. The energy dissipation takes part in terminals. Because of the energy dissipation the local temperature $T_{term}$ in terminals is higher than the temperature $T_{wire}$ of nanowires itself (Fig. 2) and a heat distribution in terminals of a nanostructure should be analyzed.

![Figure 2. Distribution of the electrical conductance and the temperature in a nanowire with a ballistic transport.](image)

In small structures a dissipated energy is quite large. For the first step of conductance quantization, $G_e = G_{E0} = 7.75 \times 10^{-5} \text{[A/V]}$, and at the supply voltage $V_{sup} = 1V$ the current in the circuit $I_1 = 72 \mu A$ ($I_2 = 134 \mu A$ for the second step of quantization). The power dissipation in terminals of nanowires is $P = I_1^2/G_{E0} = 67\mu W$ for the first step of quantization, and $P = I_2^2/2G_{E0} = 116\mu W$ for the second step. One ought to notice that the density of electric current in nanowires is extremely high. The diameter of the gold nanowire on the first step of quantization can be estimated to $D = 0.27 nm$ (the radius of a gold atom $r = 0.135 nm$), so for $I = 72 \mu A$ the current density $J = 12 \times 10^{10} \text{[A/cm}^2\text{]}$.

Silicon atom has the diameter of 0.22nm, the lattice space in Si is of 0.543nm. In an one atom layer silicon structure with $W$ width, at the temperature of 300 K transmission channels with parameters shown in Table I are formed, where $N$ is the number of channels, $R$ is the resistance of a nanostructure, $G_T$ is the thermal conductance of a nanostructure.

### Table I. Electrical Resistance and Thermal Conductance of Silicon Nanostructures

<table>
<thead>
<tr>
<th>$W$ (nm)</th>
<th>0.22</th>
<th>0.54</th>
<th>1.09</th>
<th>1.63</th>
<th>2.17</th>
<th>2.71</th>
<th>3.25</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N$</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>6</td>
<td>7</td>
</tr>
<tr>
<td>$R$ (kΩ)</td>
<td>12.9</td>
<td>6.45</td>
<td>4.3</td>
<td>3.2</td>
<td>2.6</td>
<td>2.15</td>
<td>1.84</td>
</tr>
<tr>
<td>$G_T \times 10^{-10}$ [W/K]</td>
<td>2.8</td>
<td>5.6</td>
<td>8.4</td>
<td>11.2</td>
<td>14</td>
<td>16.8</td>
<td>19.2</td>
</tr>
</tbody>
</table>

III. Measurements of Electrical Conductance

The experimental setup consisted of a pair of metallic wires (they formed a nanowire), a digital oscilloscope, a motion control system (doesn’t show on the picture) and a PC. Instruments are connected in one system using the IEEE-488 interface. The circuit was fed by the constant voltage $V_{sup}$ and measurements of current $I$ was performed. Transient effects of making contact or breaking the contact give time dependent current. Both electrodes (macroscopic wires) are made of wire 0.5 mm in diameter. All experiments were performed at room temperature and at ambient pressure.

In order to compare our results with those published before by other groups the first experiment was performed for gold wires. Even if the quantization of conductivity by $G_0 = 2e^2/h$ does not depend on the metal and on temperature, the purpose of studying quantization for different metals was to see how properties of the metal affect the contacts between wires. All measurements were carried out at room temperature.

The quantization of electric conductance depends neither on the kind of metal nor on temperature. However, the purpose of studying the quantization for different metals was to observe how the metal properties affect the contacts between wires. For nonmagnetic metals, the conductance quantization in units of $G_{E0} = 2e^2/h = (12.9 kΩ)^{-1}$ was previously observed for the following nanowires: Au-Au, Cu-Cu, Au-Cu, W-W, W-Au, W-Cu. The quantization of conductance in our experiment was evident – see Fig. 3. All characteristics showed the same steps equal to $2e^2/h$. We observed two phenomena: quantization occurred when the contact between two wires is breaking, and quantization occurred when the contact between the wires is establishing. The characteristics are only partially reproducible; they differ in number and height of steps, and in the time length. The steps can correspond to 1, 2, 3, 4, 5 or 6 quanta, as is shown in Fig. 3. The conductance quantization has been so far more pronouncedly observable for gold contacts. Fig. 3 shows an example of plots of conductance vs. time during the process of drawing a gold nanowire. More results from the experiment described above are given in Ref. [9].

IV. CONCLUSIONS

Conductance quantization has proved to be observable in a simple experimental setup, giving opportunity to investigate subtle quantum effects in both electrical and thermal conductivity. The energy dissipation in Nanowires takes part in their terminals. Because of the energy dissipation the local temperature in terminals is higher than the temperature of nanowire itself.

The potential application field of our investigation is scaling of electronic devices inside digital integrated circuits [9] and NEMS devices (Nano-Electro-Mechanical Systems). At present, microprocessors are produced in 14-nm technology (e.g. 14-nm Exynos systems-on-a-chip by Samsung or the i7-5557U by Intel). Even more, the Intel is developing the 10-nm technology for 2016 and the 5-nm technology for 2020. Electronic scaling of electronic devices inside digital integrated circuits [9] and NEMS devices (Nano-Electro-Mechanical Systems). At present, microprocessors are produced in 14-nm technology (e.g. 14-nm Exynos systems-on-a-chip by Samsung or the i7-5557U by Intel). Even more, the Intel is developing the 10-nm technology for 2016 and the 5-nm technology for 2020. Electronic devices and connecting paths in integrated circuits of such dimensions really will be nanostructures. The quantum phenomena discussed above should be taken into account at designing digital circuits of Very Large Scale of integration (VLS).

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Waldemar Nawrocki is a professor of electronics at Poznan University of Technology, Poland, where he earned a Ph.D. in technical sciences in 1981. Dr. Nawrocki also holds a D.Sc. in physics from Jena University, Germany, since 1990. His research fields are: Applications of quantum effects in metrology, Quantization of conductance in mesoscopic systems, Applications of SQUID detectors for a noise thermometry, Cryoelectronics, Measurement systems. Dr. Nawrocki published 14 books, e.g. Measurement Systems and Sensors (Artech House, Boston, 2005) and Introduction to Quantum Metrology (Springer, Heidelberg, 2015). In the period from 2006 to 2013, he organized and chaired four international conferences on quantum metrology.

Yury M. Shukrinov is a leading scientist of the Joint Institute for Nuclear Research, Dubna and professor of University Dubna, Russia. He had his PhD on Low Temperature Physics and Cryogenic Technique from Moscow State University in 1981. Today his research interests are concentrated on the condensed matter physics and theory of superconductivity, particularly, superconducting electronics, tunneling in superconducting structures and intrinsic Josephson effect. He had his second degree of Doctor of Sciences from Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research in 2014 on collective dynamics of coupled Josephson junctions in layered superconductors. He is coauthor more than 150 scientific publications.