The Kinetic Effects, Caused by Thickness Fluctuations of Quantum Semiconductor Wire

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The electrical conductivity, thermopower and thermal conductivity of semiconductor quantum wire conditioned by a random field of Gaussian fluctuations of wire thickness are theoretically determined. We present the results for cases nondegenerate and generate statistics of carriers. The considered mechanism of relaxation of the carriers is essential for sufficiently thin and clean wire from the A3B5 and A4B6 type of semiconductors at low temperatures. The quantum size effects that are typical of quasi-one-dimensional systems were revealed.

Keywords: Semiconductor quantum wire, Gaussian fluctuations of thickness, Electrical conductivity, Thermopower, Thermal conductivity.

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1. INTRODUCTION

In thin semiconductor wire quantization of electron energy spectrum leads to quantum size effects, which are found in the kinetic parameters of quasi-one-dimensional system, which are also depended on the mechanism of carriers scattering. In modern nanoelectronics technologies the influence of random field associated with fluctuations in the thickness of semiconductor quantum wires, generally speaking, cannot be ignore [1]. The aim of this work is to generalize and refine previous studies [2] the proliferation impact of such fluctuations on the basic kinetic characteristics of semiconductor quantum wire.

2. THEORETICAL MODEL

In [4] the model of semiconductor quantum wires with cross sizes, limited by thickness \( d \) (in the direction of coordinate axis \( z \)) by one-dimensional a potential pit \( V(z) \) with infinitely high walls and for the width (towards \( y \)) parabolic potential \( \beta \) \( (\beta > 0) \) are considered. The considered magnetic field \( H \) is directed along the wire (axis \( x \)); components of the vector potential of magnetic field: \( A_x = A_y = 0, A_z = H_z \).

In the mean field theory (one-electron approximations) Hamiltonian system has the form

\[
\hat{H} = \frac{\hbar^2}{2m_\perp} \Delta_z + \frac{1}{2m_\perp} \left( -i\hbar \frac{\partial}{\partial z} + \frac{e}{c} A_z \right)^2 + V(z) + \beta y^2 + U(z),
\]

where \( \Delta_z = \frac{\partial^2}{\partial z^2} + \frac{\partial^2}{\partial y^2} \), \( m_\perp = m_x = m_y = m \) - effective mass of the electron along appropriate directions, \( e \) - the absolute value of the electron charge,

\[
V(z) = \begin{cases} 0, & -d/2 \leq z \leq d/2, \\ \infty, & z < -d/2, z > d/2, \end{cases}
\]

\[
U(r_z) = a(\xi(z) - \delta(z)),
\]

\[(3)\]

- potential energy of an electron in a random field, caused by fluctuations in the thickness of the wire, \( \alpha = \partial E_\perp / \partial d \), \( E_\perp \) – the bottom of the conduction band, \( \xi(z) \) – a random functions that determine the amplitude of fluctuations on different surfaces of the wire perpendicular to the axis \( z \).

Interaction (3) of carriers with a random field is considered a disturbance which causes the quantum transitions in the translational movement along the wire (in the direction of the axis \( x \)). We confined by contribution of lower quantum size level of the electron cross motions. In approximation of account of electron states with a certain parity in the \( x \)-axis wave function of unperturbed problem is

\[
\psi_{k_x}(r) = \sqrt{\frac{2}{\pi^{1/4} \hbar d}} \exp \left( i k_x x - \frac{y^2}{2\gamma_0} \right) \cos \left( \frac{\pi}{d} z \right),
\]

where \( L \) – wire length \( (L >> d) \),

\[
\gamma_0 = \hbar^{3/4} \left[ \frac{2m}{\beta + \frac{\hbar^2 H^2}{2m c^2}} \right]^{-1/4}.
\]

The energy of an electron in a state (4):

\[
E(k_x) = \frac{\hbar^2 k_x^2}{2m} + \frac{\pi^2 \hbar^2}{2md^2} + \hbar \left[ \frac{1}{2m} \left( \beta + \frac{\hbar^2 H^2}{2m c^2} \right) \right]^{-1/2}.
\]

3. THE RELAXATION TIME

The inverse relaxation time of the electron along the wire length at the scattering of fluctuation field (3) has the form

\[
\frac{1}{\tau_x(k_x)} = \frac{2\pi}{\hbar} \sum_j \left( \frac{\langle k_x \mid \Gamma \mid k_x \rangle}{k_x} \right) \left[ 1 - \frac{k_x^2}{K_x^2} \right] \times \delta \left[ E(k_x) - E(k_x^j) \right],
\]

\[(7)\]
where double brackets \( \langle \ldots \rangle \) determine averaging over the random field. Fluctuations on different surfaces of wire are considered independent and on one surface - Gauss fluctuations:

\[
\langle (\xi (\mathbf{r}_1), \xi (\mathbf{r}_2)) \rangle = \delta_{ij} \Lambda_i^2 \exp\left[ -\frac{(\mathbf{r}_{1i} - \mathbf{r}_{2i})^2}{2 \Lambda_i^2} \right],
\]

\[
\langle \xi (\mathbf{r}_i) \rangle = 0, i, j = 1, 2.
\]

After calculating (7) with (3) and (8) we find a general expression for the relaxation time [2]

\[
\frac{1}{\tau_n(k_i)} = \frac{\alpha^2 m n k_i^2}{\hbar^2} \sum_{\Delta_i \Lambda_i} \xi_i^2 \langle \mathbf{k}_i \rangle dk_i,
\]

where \( f_\circ = \left\{ \exp \left[ \frac{\epsilon - \mu}{k_B T} \right] + 1 \right\}^{-1} \) - distribution function of the Fermi-Dirac, \( \epsilon = \hbar^2 k_i^2 / 2m, \mu \) - chemical potential, measured from the quantum-dimensional level of movement of electrons across the wire, \( 2 \sum \xi_i^2 = N \) - the total number of electrons in a wire.

In [2], taking into account the general expression for the relaxation time (9), a bit bulky finial expressions for conductivity \( \sigma_n \), found from (10) were obtained and analyzed for arbitrary values of \( \Delta_i, \Lambda_i \), magnetic field \( H \) and temperature \( T \).

Dependecies of \( \sigma_n \) on longitudinal magnetic field \( H \) are associated with compression of wave function of electrons across the wire (along the axis y) and are determined by factor \( \frac{\gamma_k^2 (H) + \Lambda_i^2}{\Lambda_i^2} \) (See. (5)). At \( \gamma_k^2 (H) \ll \Lambda_i^2 \) and extremely strong magnetic field \( \epsilon^2 H^2 / 2m, \epsilon^2 \gg \beta \), this leads to the appearance in on the factor \( H^{-1/2} \).

For simplicity in (9) the case \( H = 0 \) \( \Lambda_1 = \Lambda_2 = \Lambda \) was considered. Then for relaxation time \( \tau_n(\epsilon) \) of an electron with energy \( \epsilon \), we have:

\[
\tau_n(\epsilon) = B \epsilon^{1/2} \exp(\gamma \epsilon),
\]

where

\[
B = \frac{\hbar^2}{2 \pi} \left[ \alpha^2 (\pi m)^{1/2} (A_1 + A_2) \right],
\]

\[
A_i = \frac{(\Lambda_i \Lambda_i)^2}{\gamma_k^2 + \Lambda_i^2}, \quad \gamma = 4 m \Lambda^2 / \hbar^2.
\]

According to (10) conductivity can be written in the form [3]:

\[
\sigma_n = e^2 K_0, \quad (14)
\]

where

\[
K_0 = \frac{2^{3/2}}{\pi \hbar m^{3/2} n^2} \int_0^{\tau_n(\epsilon)} \frac{d \epsilon}{\sqrt{\epsilon}} \exp\left[ -\frac{(\epsilon - \mu)^2}{2 \hbar^2} \right]. \quad (15)
\]

For nondegenerate case of semiconductor wire including (11) – (13) we obtain:

\[
\sigma_n = \frac{2 \hbar \epsilon^2 n}{\pi \alpha^2 m^{3/2}} \left( 1 - \gamma k_B T \right)^{1/2} \left( A_1 + A_2 \right)^{-1}, \quad (16)
\]

where \( n = N/L \) – the number of electrons per unit length. Equation (16) fair when \( 1 - \gamma k_B T > 0 \) and \( \hbar^2 (1 - \gamma k_B T)^{2/3} / 2mk_B T^2 > 1 \), where \( l \) – is the lattice constant along the axis of the wire. The first condition associated with that the relaxation time \( (9), (11) - (13) \) increases exponentially with the energy of the electron, and Maxwell distribution decreases exponentially. Therefore, for the efficiency of scattering by Gauss fluctuations is significantly that de Broglie "heat" wavelength of the charge carrier exceeded the value of the correlation radius \( \Lambda \).

The second condition is associated with a choice of infinite upper limit of the integral (10), (15) and is usually performed. In the case of low temperatures and \( \gamma k_B T < 1 \) the electron mobility along the axis of the wire is \( \mu_n \propto (k_B T)^{1/2} \) which for the temperature dependence resembles a dipole scattering [4] for three-dimensional semiconductor materials.

For degenerate case and \( \hbar k_B T < \mu \) conductivity along the axis of wire including the general expression for the relaxation time (9) is

\[
\sigma_n \propto \frac{4e^2 h}{\alpha^2 m \sqrt{2\pi}} \mu \times \left[ A_1 \exp(-2k_F^2 \Lambda_1^2) + A_2 \exp(-2k_F^2 \Lambda_2^2) \right]^{-1},
\]

where \( k_F^2 = (2m / \hbar^2) \mu \). Temperature dependence \( \sigma_n \) is determined of chemical potential of one-dimensional electron gas

\[
\mu \approx \mu_0 \left[ 1 + \pi^2 \left( \frac{k_F T}{\mu_0} \right)^2 \right]^{-1},
\]

\[
\mu_0 = \frac{\hbar^2}{8 m} \left( \frac{n}{\pi} \right)^2.
\]

According to calculations for wires A3BS materials (eg, GaAs [2]) and A4B6 mechanism of relaxation of charge carriers at random roughness of boundaries is essential at low temperatures \( k_B T < \hbar^4 / 4m \Lambda^2 \) for clean enough samples and nanometer thicknesses.

The effects of localization type [5], which arising in quasi-one-dimensional systems in heavy clutter (or at very high concentrations of impurities) which can not be explained within the theory of weak scattering in our work are not considered. So we obtained temperature dependence of conductivity significantly different from the consequences of the theory of localization [5].
5. THERMOPOWER

According to kinetic Boltzmann equation thermoelectric power $S_{xx}$ can be written [3, 6] in view

$$ S_{xx} = -\frac{1}{e^T} K_0^{-1} K_1, $$

(20)

where $K_0$ is determined by formula (15),

$$ K_1 = \frac{2^{3/2}}{\pi \hbar m^{1/2}} \int_0^\infty \tau_0 (\epsilon) \left( \frac{\partial f_0}{\partial \epsilon} \right) (\epsilon - \mu) \epsilon^{1/2} d\epsilon. $$

(21)

After the resuffle in the (20) formulas (15) and (21) with (11) we obtain [4] at $\gamma k_B T < 1$:

$$ S_{xx} = -\frac{1}{e^T} \left( \frac{F_{xy}}{F_{xy}} - \mu \right), $$

(22)

where

$$ F_{xy} = \int_0^\infty \tau_0 (\epsilon) \epsilon^{1/2} d\epsilon, \quad F_{xy} = \int_0^\infty \left( \frac{\partial f_0}{\partial \epsilon} \right) \epsilon^{1/2} d\epsilon. $$

(23)

For nondegenerate statistics of carriers $f_0 = \exp[(\epsilon - \mu)/k_B T]$ from (22) and (23) we find at $1 - \gamma k_B T > 0$

$$ S_{xx} = -\frac{k_B}{e} \left( \frac{2}{1 - \gamma k_B T} - \frac{\mu}{k_B T} \right), $$

(24)

where the chemical potential of one-dimensional electron gas

$$ \mu = k_B T \ln \left[ \frac{\hbar n}{\pi 2m k_B T} \right]^{1/2}. $$

(25)

Due to summand $2(1 - k_B T) - 1$ there is the possibility of increasing thermoelectric power for onedimensional quantum wire.

For the case of highly degenerate one-dimensional electron gas at $k_B T < \mu$, using the standard for this limiting case approach [5], we get

$$ S_{xx} = \frac{\pi^2}{3e} k_B \left( \frac{k_B T}{\mu} \right) (1 + \mu), $$

(6)

where the chemical potential $\mu(T)$ determined by question (18), (19). Due to summand $\gamma \mu$ in (26) we have a theoretical possibility to increase the value of thermoelectric power for considered one-dimensional case.

6. THERMOPOWER

According to [3, 6] coefficient of thermal conductivity is determined by the formula:

$$ \kappa = \frac{1}{T} \left( K_2 - \frac{K_2}{K_0} \right), $$

(27)

where

$$ K_2 = \frac{2^{3/2}}{\pi \alpha m^{1/2}} \int_0^\infty \tau_0 (\epsilon) \left( \frac{\partial f_0}{\partial \epsilon} \right) (\epsilon - \mu) \epsilon^{1/2} d\epsilon. $$

(28)

For nondegenerate system of charge carriers for $1 - \gamma k_B T > 0$ we have:

$$ K_0 = \frac{2\hbar^2 n}{\pi \alpha m^{1/2}} \left( k_B T \right)^{1/2} \left( A_1 + A_2 \right)^{-1}, $$

(29)

$$ K_1 = \left( \frac{F_{xy}}{F_{xy}} - \mu \right) K_0, $$

(30)

$F_{xy}$ and $F_{xy}$ we find from (23).

$$ K_2 = \frac{2\hbar^2 n}{\pi \alpha m^{1/2}} \left( k_B T \right)^{1/2} \times $$

$$ \times \left[ \frac{6(k_B T)^2}{(1 - \gamma k_B T)} - \frac{4\mu k_B T}{(1 - \gamma k_B T)} + \mu^2 \right] \left( A_1 + A_2 \right)^{-1}. $$

(31)

According to formulas (29) – (31) and (27) we obtain the final result for the thermal conductivity of semiconductor quantum wire caused by fluctuations in the thickness:

$$ \kappa = \frac{1}{T} \left[ \frac{2\hbar^2 n}{\pi \alpha m^{1/2}} \left( k_B T \right)^{1/2} \times $$

$$ \times \left[ \frac{2(k_B T)^2}{(1 - \gamma k_B T)} - \frac{2\mu k_B T}{(1 - \gamma k_B T)} + \frac{3}{4} \mu^2 \right] \left( A_1 + A_2 \right)^{-1} \right]. $$

(32)

where $\mu$ – chemical potential one-dimensional electron gas (see. (25)).

Using (16) and (32), we find the relation

$$ \frac{\kappa}{\sigma n T} = \frac{2}{\alpha m^{1/2}} \left( \frac{k_B T}{e} \right)^2 \times $$

$$ \times \left[ \frac{1}{(1 - \gamma k_B T)^2} - \frac{\mu}{k_B T (1 - \gamma k_B T)} + \frac{3}{8} \left( \frac{\mu}{k_B T} \right)^2 \right], $$

(33)

which shows that Wiedemann-Franz law holds only at $\gamma k_B T << 1$ and $\mu << k_B T$.

For case of strongly degenerate electron gas at $k_B T << \mu$ and $A_1 = A_2 = \Lambda$ we have:

$$ K_0 = \frac{2\hbar^2 n}{\pi \alpha m^{1/2}} \left( A_1 + A_2 \right)^{-1} e^{\gamma \mu}, \quad \sigma_n = e^2 K_0, $$

(34)

$$ K_1 = \frac{\pi^2}{3} \left( k_B T \right)^2 \frac{1}{\mu} \left( 1 + \gamma \mu \right) K_0, $$

(35)

$$ K_2 = \frac{2^{3/2}}{\pi \alpha m^{1/2}} \hbar \mu \left( k_B T \right)^{1/2} \left( A_1 + A_2 \right)^{-1} e^{\gamma \mu}. $$

(36)

From (27) and (34) – (36) obtain
Based on the expressions of the relaxation time of charge carriers, conductivity, thermoelectric power and thermal conductivity of quantum semiconductor wire it is shown that the mechanism of relaxation is caused by a random field Gauss fluctuations in the thickness of wire may be effective for sufficiently thin and clean wire from the material A3B5 and A4B6 in thicknesses of nanometric size. The possibility of increasing some kinetic parameters of quasi-one-dimensional systems is revealed.

7. SUMMARY

Kineticheskie effekty, obuslovennye fluktatsiyami toshchnosti kvantovoy poluprovodnikovoy provolok

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Теоретично визначено електропроводність, термоелектричність та теплопроводність квантового полупроводникового проводника. Розглянутий механізм релаксації носіїв заряду є характерним для квазіодновимірних систем.

Ключові слова: Квантовий полупроводниковий проводник, Гауссовські флуктуації товщини, Електропроводність, Термо ЕДС, Теплопроводність.

Кінетичні ефекти, обумовлені флуктуаціями товщина квантового напівпровідникового дроту

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