Effect of short-range impurities on low-temperature conductance and thermopower of quantum wires

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The electron transport through the parabolic quantum wire placed in longitudinal magnetic field in the presence of the system of short-range impurities inside the wire is investigated. Using approach based on the zero-range potential theory we obtained an exact formula for the transmission coefficient of the electron through the wire that allows to calculate such the transport characteristics as the conductance and differential thermopower. The dependencies of conductance and thermopower on the chemical potential and magnetic field are investigated. The effect of elastic scattering due to short-range impurities on low-temperature conductance and thermopower is studied. It was shown that the character of the electron transport essentially depends on the position of the every scattering center. The presence even isolated impurity leads to destruction of conductance quantization. In some cases it is possible that thermopower can change the sign in dependence on chemical potential and magnetic field.

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1. INTRODUCTION

Electron transport in mesoscopic systems has many long years attracted attention, both theoretical and experimental. There are many interesting phenomena in this area. The effect of conductance quantization has first observed in the narrow constriction that connect two large areas of two-dimensional electron gas (2DEG) in high-mobility GaAs-AlxGa1−xAs heterostructures. The above discovery has stimulated a whole series of theoretical works where the various models of confinement potential have been used: an infinitely long waveguide with constant cross section, saddle-point potential and other ones. All these papers based on Landauer-Büttiker transport approach.

The character of conductance quantization in quasi-one-dimensional (Q1D) systems depends on the geometry of the quantum wire, on its length and width. Applied magnetic field \( B \) plays the key role in such a system. A magnetic field enhances lateral confinement so that by varying \( B \) we can alter the effective geometrical size of the system, and hence the functional dependence of the conductance on the field \( B \). In particular, by varying \( B \) one can change the parameters of the conductance quantization steps (length of the conductance plateau). The parameters of the conductance quantization depend sufficiently not only on magnitude of magnetic field but also on its direction.

However, the conductance quantization is very sensitive to electron scattering. There are three principal type of scattering that can lead to destruction of the conductance quantization: (i) scattering in the region of the contact of wire with electron reservoirs, (ii) electron scattering on rough walls of the wire and (iii) impurity scattering inside the Q1D wire (see, for instance, Refs. and references therein). Interference of electron waves due to every above-mentioned types of scattering leads to oscillatory dependence of conductance on Fermi energy.

Simultaneous consideration of every above-mentioned scattering factors is the sufficiently complicated problem. Therefore in the present paper, we shall focus our attention only on the effect of impurity scattering.

Note that all previous papers concerned consideration of the effects of the impurities on the electron transport in Q1D systems had some limitations: as a rule the number of impurities was equal to unity. Both experimental and theoretical study of the effect of impurity on quantized conductance of Q1D wire shows that even isolated impurity can lead to fundamental change of the conduction character.

Large number of works were devoted to conductance of quantum wires in the case when an isolated short-range impurity contained inside the wire. It was found that the main features of the conductance \( G \) are downward dips in the graph of \( G \) vs Fermi energy below the bottom of each transverse mode in the case of infinite rectilinear waveguide and a resonance peak below the first quantized step in the case of a saddle-point potential of quantum point contact (QPC) due to resonant transmission through bound state. The effect of a finite-range scatterer was discussed in Refs.

Besides conductance \( G \), thermopower \( S \) is another transport property of Q1D systems in which quantization effect manifests. It was first shown theoretically by Streda that in narrow constriction the thermopower \( S \) exhibits oscillatory dependence as a function of Fermi energy. It was shown that peak values of \( S \) are quantized, given by \( \ln 2/(i+1/2) \) (in units \( k_B/e \)). These peaks occur when the Fermi energy \( \mu \) is close to edge of \( i \)th transverse subband (\( i = 1, 2, ... \)), that is the peak in thermopower corresponds to the quantized conductance threshold.
The above-mentioned quantum oscillations have been demonstrated in experiment. Later theoretical studies confirm the results of Streda and moreover dependencies of thermopower on magnitude and direction of applied magnetic field were studied.

However, we know only one paper where effect of impurity on low-temperature thermopower was investigated. The existence of negative thermopower due to backscattering of applied magnetic field were studied in experiment. The above-mentioned quantum oscillations have been confirmed the results of Streda and moreover dependencies of thermopower on magnitude and direction of applied magnetic field were studied.

We present the theory of the quasi-ballistic electron transport in quantum wire for the case of any finite number of scattering centers. The aim of present work is to study the effect of elastic scattering due to \( N \) short-range impurities on the such transport characteristics as conductance and thermopower of quantum wire. We include in consideration only effects those deal with impurity scattering excluding other scattering types.

The paper is organized as follows. In Sec. 2 we describe the model and Hamiltonian and find analytical formula for conductance and thermopower and the model and Hamiltonian and find analytical formula for conductance and thermopower of quantum wire. We in-section range impurities on the such transport characteristics as well-known form.

The corresponding wavefunctions in cylindrical coordinates \( r = (\rho, \varphi, z) \) are given by

\[
E_{mnk} = \frac{\hbar \omega_c}{2} m + \frac{\hbar \Omega}{2} (n + |m| + 1) + \frac{\hbar^2 k^2}{2m^*},
\]

where \( \Omega = \sqrt{\omega_c^2 + 4 \omega_0^2}, \omega_c = |e| B/m^* c \) is the cyclotron frequency, \( m = 0, \pm 1, \pm 2, \ldots, n = 0, 1, 2, \ldots, k \) is the electron wavevector in wire’s axis direction.

The corresponding wavefunctions in cylindrical coordinates \( r = (\rho, \varphi, z) \) are given by

\[
\psi_{mnk}^0 = R_{mn}(\rho) e^{im\varphi} e^{ikz},
\]

where \( R_{mn}(\rho) = C_{mn} \rho^{|m|} \exp(-\rho^2/4l_0^2) L_n^{\text{in}}(\rho^2/2l_0^2), \)

and

\[
C_{mn} = \frac{1}{\binom{m}{2}} \left[ \frac{n!}{(n + |m|)!} \right]^{1/2},
\]

with

\[
R_{mn}(\rho) = C_{mn} \rho^{|m|} \exp(-\rho^2/4l_0^2) L_n^{\text{in}}(\rho^2/2l_0^2),
\]

and

\[
C_{mn} = \frac{1}{\binom{m}{2}} \left[ \frac{n!}{(n + |m|)!} \right]^{1/2},
\]

where \( L_n^{\text{in}}(x) \) are generalized Laguerre polynomials, \( l_0 = \sqrt{\hbar/m^* \Omega} \). It is evident the normalization of the longitudinal part of the wavefunction can be chosen in arbitrary form, because it is unimportant to find transmission coefficients.

It is well-known that the Green function \( G(\mathbf{r}, \mathbf{r}'; E) \) can be represented for Q1D system in the following form

\[
G(\mathbf{r}, \mathbf{r}'; E) = \sum_\alpha G_z(z, z'; E - E_\alpha) \psi_\alpha(x, y) \psi_\alpha^*(x', y'),
\]

where \( \psi_\alpha(x, y) \) is the transverse part of Q1D wavefunction, \( E_\alpha \) is the bottom of transverse subband and

\[
G_z(z, z'; E) = \frac{im^*}{\hbar^2} e^{ik|z - z'|}
\]

is the Green function of the operator \( H_z = -(\hbar^2/2m^*) \partial^2/\partial z^2 \).

In the case of our model above-mentioned representation leads to the following form of Green’s function of the unperturbed Hamiltonian \( H \), that is necessary to solve the present problem in some analogy with Ref.13.

\[
G(\mathbf{r}, \mathbf{r}'; E) = \frac{im^*}{2\pi \hbar^2} \sum_{n=0}^{\infty} \sum_{m=-\infty}^{\infty} R_{mn}(\rho) R_{mn}(\rho')
\]

\[
\times e^{ik_{mn}|z - z'| + im(\varphi - \varphi')} k_{mn},
\]

where \( \hbar k_{mn} = \sqrt{2m^*(E - E_{mn})} \).

Let us find the exact solution of Schrödinger equation for the Hamiltonian \( H = H_0 + U(r) \), where \( U(r) \) is the potential created by \( N \) short-range impurities. It is rightful to use the zero-range potential for modelling short-range impurities as long as the impurity range is shorter than all other relevant length scales in the problem. Let us remind that above potential describes only spherically-symmetric s-scatterer and can be expressed as the boundary condition for the wavefunction.

This approach allows to find exact solution of Schrödinger equation and therefore we can find the exact expressions for transmission coefficients that in one’s turn allows to find conductance and thermopower. Here we use only some consequences of above-mentioned
approach. The asymptotic of the wave-function in the vicinity of the each impurity point $\mathbf{q}_j$ does not depend on any smooth potential (in our case it is the confinement potential) and has the form

$$
\psi(r)|_{r \to \mathbf{q}_j} = C_j \left( \frac{1}{|r - \mathbf{q}_j|} - \frac{1}{a_j} \right) + O(|r - \mathbf{q}_j|), \quad (6)
$$

where $C_j$ is the some constant, $a_j$ is the scattering length for impurity that locates at the point $\mathbf{q}_j$.

The zero-range potential theory allows us to represent the solution of Schrödinger equation with Hamiltonian $H$ in terms of the Green’s function $G(\mathbf{q}_i, \mathbf{q}_j; E)$.

$$
\psi(r) = \psi^0(r) + \sum_{j=1}^{N} \alpha_j G(r, \mathbf{q}_j; E), \quad (7)
$$

Considering the asymptotic of the eigenfunction near each point $\mathbf{q}_j$ one can find the system equation for $\alpha_j$ determination

$$
\sum_{i=1}^{N} \alpha_i (Q_{ij} + \Lambda_j \delta_{ij}) + \psi^0(\mathbf{q}_j) = 0, \quad j = 1, \ldots, N. \quad (8)
$$

where $\Lambda_j$ is the parameter that characterizes the strength of the zero-range potential at the point $\mathbf{q}_j$ and $\delta_{ij}$ is the Kronecker delta, with respect to the scattering length $a_j$, is given by equation $\Lambda_j = m^*/2\pi \hbar^2 a_j$. Negative $\Lambda$ corresponds to presence of the bound state for isolated impurity (whereas for the case $N > 1$ bound states can exist for either sign of $\Lambda$). Large values of $|\Lambda|$ correspond to weak impurity.

The elements of so-called Krein’s $Q$-matrix are given by

$$
Q_{ij}(E) = \begin{cases} 
G(\mathbf{q}_i, \mathbf{q}_j; E), & i \neq j, \\
\lim_{r \to \mathbf{q}_i} \left[ G(r, \mathbf{q}_j; E) - \frac{m^*}{2\pi \hbar^2} \frac{1}{|r - \mathbf{q}_j|} \right], & i = j.
\end{cases} \quad (9)
$$

The convergence of $Q_{ij}$ was demonstrated in Ref.34 by means of the integral representation.

The asymptotic expansion for $G(r, \mathbf{q}_i; E)$ at $r \to \mathbf{q}_i$ can be found only in some limiting cases. However the impurity scattering is more sufficient when the impurities are located near wire’s axis33. In this case we can use the following formula for $Q_{ij}(E)$ determination

$$
Q_{ij}(E) = \lim_{r \to \mathbf{q}_j} [G(r, \mathbf{q}_j; E) - G(r, \mathbf{q}_i; E_0)] + C, \quad (9)
$$

where $E_0$ is the some fixed value of the energy, the constant $C$ can be determined considering case when the asymptotic of Green’s function is definite. It is conveniently to put $E_0 = 0$. In this case $C$ is given by $C = (m^*/2\sqrt{2\pi \hbar^2}) \zeta(1/2; 1/2)$, where $\zeta(s; x)$ is the generalized Riemann zeta function.

The solution of system of equations (6) leads us to the eigenfunctions of the Hamiltonian $H$ (with the same energy that for $\psi^0_{mnk}$)

$$
\psi(r) = \psi^0(r) - \sum_{i,j=1}^{N} [Q(E) + i\Lambda]^{-1} \psi^0(\mathbf{q}_j) G(r, \mathbf{q}_i; E).
$$

Here $E$ is the unitary matrix $N \times N$, $\Lambda = (\Lambda_1, \ldots, \Lambda_N)^T$ ($T'$ denotes the transposed vector), $A^{-1}$ is the inverse matrix for $A$.

It is evident that far from impurities ($z \to \infty$) the following expansion is right

$$
\psi_{mnk}(r) = \sum_{m'n'} t_{mn,m'n'} \psi^0_{m'n'}(r), \quad (11)
$$

where $t_{mn,m'n'}$ is the transmission amplitude from incident mode $nn$ to transmitted mode $m'n'$ ($k' = k_{m'n}$), and the summation in Eq. (11) is over all transmitted modes ($E > E_{mn}$, for real $k_{mn}$) because the modes which correspond to imaginary $k_{mn}$ rapidly decay on large $z$.

From Eqs. (10,11) we find for the transmission amplitude

$$
\begin{equation}
\begin{aligned}
& t_{mn,m'n'} = \delta_{m'n'} \delta_{mn} - \frac{im^*}{2\pi \hbar^2 k_{m'n'}} \\
& \times \sum_{i,j=1}^{N} \left( (\psi^0_{m'n'k'}(\mathbf{q}_i))^* [Q(E) + i\Lambda]^{-1} \psi^0_{mnk}(\mathbf{q}_j) \right),
\end{aligned} \quad (12)
\end{equation}
$$

It is conveniently to write Eq. (12) in the matrix form

$$
\begin{equation}
\begin{aligned}
& t_{mn,m'n'} = \delta_{m'n'} \delta_{mn} - \frac{im^*}{2\pi \hbar^2 k_{m'n'}} \hat{\psi}_1 \hat{F} \hat{\psi}_2,
\end{aligned} \quad (13)
\end{equation}
$$

where $\hat{\psi}_1 = [\psi^0_{m'n'k'}(\mathbf{q}_1), \ldots, \psi^0_{m'n'k'}(\mathbf{q}_N)], \quad \hat{F}$ is the inverse matrix for $[Q(E) + i\Lambda]$, and $\hat{\psi}_2 = (\psi^0_{mnk}(\mathbf{q}_1), \ldots, \psi^0_{mnk}(\mathbf{q}_N))^T$.

The first term in Eq. (12) corresponds to ballistic transmission of electrons through the wire when the inter-subband transitions are forbidden. The second term corresponds to mode-mixing due to impurity scattering.

3. CONDUCTANCE AND THERMOPOWER

Accordingly to Landauer-Büttiker approach the two-probe Landauer conductance $G$ is given by

$$
G = \frac{e^2}{\pi \hbar} \int_{0}^{\infty} dE \left( -\frac{\partial f}{\partial E} \right) \sum_{\alpha,\alpha'} T_{\alpha,\alpha'}(E), \quad (14)
$$

where $f(z) = [e^{z-\mu}/T + 1]^{-1}$ is the Fermi distribution function, $\mu$ is the chemical potential.

For the case of thermoelectric transport the differential thermopower $S$ is given by the formula

$$
S = \frac{k_B}{e} \int_{-\infty}^{\infty} dE \left( \frac{-\partial f}{\partial E} \right) \frac{E - \mu}{\int_{-\infty}^{\infty} dE \left( -\frac{\partial f}{\partial E} \right) \sum_{\alpha,\alpha'} T_{\alpha,\alpha'}(E)}. \quad (15)
$$

The transmission coefficients which corresponds to the electron transition from transverse sub-band $\alpha$ to sub-band $\alpha'$ are

$$
T_{\alpha,\alpha'} = \frac{k_{\alpha'}}{k_{\alpha}} |t_{\alpha,\alpha'}|^2. \quad (16)
$$
For the case of comparatively low temperatures \((T \lesssim 5K)\) the so-called Mott formula is a good approximation for thermopower\(23\):

\[
S^M = \frac{k_B}{e} \frac{\pi^2 T}{3} \partial \ln G(\mu, T). \tag{17}
\]

For the case of the ultra-low temperatures \((T \lesssim 1K)\) there are more rough approximation. In this case Eq.\(17\) include \(G(\mu, T = 0)\). One can use this approximation in order to analyze impurity-assisted features in thermopower because they have a place at ultra-low temperatures. This approximation allows to analyze the low-temperature thermopower except the points in vicinity of conductance threshold where the zero-temperature conductance has the breakdown of the derivative on chemical potential.

Combining the Eqs.\(16),\(14\) and \(12\) we can calculate the quasi-ballistic conductance of quantum wire. Let us consider numerically the case of a perfect wire without impurities. From now on we use for electron effective mass \(m^*=0.067m_e\).

On the Fig.\(1\) the conductance of quantum wire that contains \(N\) impurities \((N = 1, 2, 3)\) is plotted. The various curves plotted for various quantity, strength and spatial distribution of impurities. One can see from Fig.\(1\) that conductance crucially depend on the position of every scattering center, its quantity and strength.

\[
\text{FIG. 1: Zero-temperature conductance as a function of Fermi energy plotted for various number, strength and spatial distribution of impurities. Dashed lines correspond to ballistic conductance of the perfect wire without impurities.} \quad \omega_0 = 10^{13}s^{-1}, \quad B = 1T.
\]

The analysis shows that \(G\) equals \(n(e^2/\pi \hbar)\) whenever the Fermi level is at the band bottom of the \((n+1)\)th subband, irrespective of the strength and location of the scatterers. And there is the zero of upper-mode transmission coefficient when the Fermi energy tends to \((E_{mn}+0)\) for any strength of the scatterers. For the purpose of comparison, the perfect-wire results are also plotted near all lines and they are indicated by dashed lines.

Taking into account that all character features of impurity-assisted thermopower appear at ultra-low temperature we can use the Cutler-Mott type formula (where zero-temperature conductance) everywhere except for the thresholds of conductance quantization where conductance-derivative undergoes the breakdown.

\[
\text{FIG. 2: Low-temperature thermopower as a function of Fermi energy plotted for various number, strength and spatial distribution of impurities. Dashed lines correspond to thermopower of the perfect wire without impurities. All parameters are the same as in Fig.\(1\).}
\]

One can see from Fig.\(2\) that thermopower \(S\) as the conductance \(G\) crucially depends on the position of every scattering center, its quantity and strength.

One can see that there is negative \(S\) at \(\mu\) that corresponds negative tilt of the curve \(G(\mu)\).

It is well-known that even single impurity influences hardly on the carrier transport through one-dimensional system and it can even lead to destruction of conductance quantization. For the case of single impurity the Krein’s \(Q\)-matrix is the scalar function and therefore we can find the exact formula for conductance at temperature \(T = 0\):

\[
G(\mu, T = 0) = \frac{\mathcal{N}(\mu)}{G_0} = \frac{\text{Im}^2 \mathcal{Q}(\mu)}{|\mathcal{Q}(\mu) + \Lambda|^2}. \tag{18}
\]

Here \(\mathcal{N}(\mu)\) is the number of transverse-quantization subband under the Fermi energy and \(G_0 = e^2/\pi \hbar\) is the conductance quantum. In Eq.\(18\) \(\mathcal{N}(\mu)\) describes the step-like dependence of ballistic conductance at \(T = 0\). For the case of one impurity we have downward dips near the thresholds in the graph of \(G\) vs Fermi energy (see Fig.\(1\)) (if bound state center exist, \(\Lambda < 0\)). In opposite case \((\Lambda > 0)\) the dependence \(G(\mu)\) is monotonic but it is not step-like.

The energies for which \(\text{Im}Q(\mu) = 0\) corresponds full transmission. And case when \(\text{Re}Q(\mu) + \Lambda = 0\) corresponds to the conductance minima \(G/G_0 = \mathcal{N}(\mu) - 1\).

The solution of above equation \(\text{Re}Q(E_0) + \Lambda = 0\) corresponds to a first approximation for energy of quasi-bound-state \(E - \mathcal{G}I\) on the complex energy plain, where \(\mathcal{G}\) determines width of the quasi-bound level.

For the case of several impurities \((N > 1)\) there are the strong dependence of transmission coefficients on the distance between each pair of impurity centers \(|q_i - q_j|\) \((i, j = 1, ..., N)\). Thus we have the strong dependence of \(G\) and \(S\) on position of each impurity \(q_i\).

4. SUMMARY

We present the exact solution for the problem of the transmission of charge-carrier through the quantum wire that contain the system of short-range impurities. Accordingly the Landauer–Buttiker approach conductance and thermopower of above system are investigated. It is obviously that in general, conductance \(G\) is lowered due to impurity scattering. The interference phenomena in transmission and existence of the negative thermopower were shown.

Note that in the case of two impurities the distance \(|q_1 - q_2|\) is equal to wire’s length one can speak about modelling of the weak scattering in the region of wire-reservoir contacts.

Let us note that for the case constriction model there are not limitation on the electron spectrum from the bottom\(19\) in contrast to the case of uniform wire. That is why the level of bound state on the impurity is in continuous spectrum and it is possible the resonant transmission.

Note that \(s\)-scattering can not explain all features of the scattering in Q1D systems, but on the whole this one is in good qualitative agreement with experimental data.
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