

Quantization of the conductance of a three-dimensional quantum wire in the presence of a magnetic field

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We study the ballistic transport in a three-dimensional quantum wire subjected to a uniform magnetic field of an arbitrary direction. The case of an elliptic cross section of the wire is considered. The temperature smearing of conductance quantization of the wire is analyzed.

I. INTRODUCTION

The conductance of a three-dimensional quantum wire is a steplike function of the electron Fermi energy.^{1,2} The height of each step is multiple of the conductance quantum $G_0 = 2e^2/h$. Such a quantization of the conductance takes place for the wire with the cross section of the order of the Fermi wavelength.

The two factors have great influence on the effect of the conductance quantization, which arises from the ballistic electron transport. On the one hand, it is the temperature of the electron gas, which smears the quantization steps (thus the effect of conductance quantization is observed at very low temperatures $T \leq 1$ K). On the other hand, the influence of the geometry of a quantum wire on the ballistic electron transport plays a very important role.³ Especially, the finiteness of the length of the wire leads to the backscattering of electron modes in the nanostructure; this gives spikes on the plot of $G(\varepsilon)$ near the thresholds of the steps.⁴ In addition, the conductance quantization is very sensitive to the boundary conditions at junctures of the wire with the electron reservoirs.⁵ As was shown,⁶⁻⁸ if the cross section varies with the length then the width of each plateau varies with ε .

Because the exact form of the confinement potential for real systems is not determined experimentally, different model potentials are employed in theoretical investigations. Especially, the waveguide with the constant cross section,^{9,10} the parabolic potential,¹¹⁻¹³ and the potential of a quantum constriction¹⁴⁻¹⁸ was used for this purpose. However, as shown,¹⁹ the simple parabolic potential is better inscribed in the self-consistent scheme taking into consideration the effects of the Coulomb interaction. A uniform magnetic field \mathbf{B} applied to the wire leads to new physical phenomena. There exists two reasons for this. On the one hand, a quantizing magnetic field amplifies the lateral confinement of electrons. On the other hand, if the field is tilted at the axis of the wire, the hybrid bindings arise along and across the wire.²⁰ This leads to the strong dependence of the conductance on the orientation of the magnetic field. Note that the effect of the field inclination on the conductance for a quantum constriction has been studied in Refs. 21 and 22. In mentioned papers the field \mathbf{B} is parallel to a symmetry plane of the confining potential of the system. It should be pointed out that the presence of one impurity charge or more leads to the reflection of electron modes. Such reflection gives spikes on the curve $G(\varepsilon)$ near the thresholds of the conductance steps.^{23,24} In this paper, we study the ballistic electron trans-

port in a quantum wire with the elliptic cross section using the asymmetric parabolic confining potential,

$$V(x,y) = \frac{m^*}{2} (\Omega_x^2 x^2 + \Omega_y^2 y^2). \quad (1)$$

Here Ω_x, Ω_y are the effective frequencies of the potential and m^* is the effective electron mass. In this model the characteristic lengths $l_j = \sqrt{\hbar/4m^* \Omega_j}$ ($j=x,y$) are equal to the semiaxes of the elliptic cross section of the wire. The magnetic field $\mathbf{B} = (B_x, B_y, B_z)$ is tilted at the arbitrary angle to the wire. Effects of scattering on the impurities and the reflection of electron modes from boundary between the wire and the electron reservoir are not considered.

II. SPECTRUM OF THE ELECTRONS IN THE WIRE IN THE PRESENCE OF A MAGNETIC FIELD

We take the vector potential \mathbf{A} of the tilted magnetic field \mathbf{B} in the form $\mathbf{A} = (0, B_z x, B_x y - B_y x)$. Then the one-electron Hamiltonian is given by the formula

$$H = H_0 + \frac{1}{2m^*} \left(p_z - \frac{e}{c} B_x y + \frac{e}{c} B_y x \right)^2 + V(x,y), \quad (2)$$

where the two-dimensional Landau Hamiltonian H_0 has the form

$$H_0 = \frac{1}{2m^*} \left[p_x^2 + \left(p_y - \frac{e}{c} B_z x \right)^2 \right]. \quad (3)$$

We denote $\omega_j = eB_j/m^*c$ ($j=x,y,z$) and introduce the notation

$$W = p_z(x\omega_y - \omega_x y) + \frac{m^*}{2} [(\Omega_x^2 + \omega_y^2)x^2 + (\Omega_y^2 + \omega_x^2)y^2 - 2\omega_x\omega_y xy]. \quad (4)$$

In the formula (4) we may eliminate the linear members with the help of the parallel translation: $x' = x - a$; $y' = y - b$; $z' = z$, where $(a,b,0)$ is the origin of the new coordinate system (x',y',z') . The numbers a and b obey the linear system of equations:

$$\begin{aligned} m^*(\Omega_x^2 + \omega_y^2)a - m^*\omega_x\omega_y b + p_z\omega_y &= 0, \\ -m^*\omega_x\omega_y a + m^*(\Omega_y^2 + \omega_x^2)b - p_z\omega_x &= 0. \end{aligned} \quad (5)$$

From Eq. (5) we obtain the following expressions:

$$a = -\frac{p_z \omega_y \Omega_y^2}{m^*} (\Omega_x^2 \Omega_y^2 + \omega_x^2 \Omega_x^2 + \omega_y^2 \Omega_y^2)^{-1},$$

$$b = \frac{p_z \omega_x \Omega_x^2}{m^*} (\Omega_x^2 \Omega_y^2 + \omega_x^2 \Omega_x^2 + \omega_y^2 \Omega_y^2)^{-1}. \quad (6)$$

In the coordinate system (x', y', z') , the Hamiltonian (2) has the form

$$H' = H'_0 + W'(x', y') + \frac{p_z^2}{2M}. \quad (7)$$

Here

$$M = m^* [1 + (\omega_x / \Omega_y)^2 + (\omega_y / \Omega_x)^2],$$

$$W'(x', y') = \frac{m^*}{2} [(\Omega_x^2 + \omega_y^2)x'^2 + (\Omega_y^2 + \omega_x^2)y'^2 - 2\omega_x \omega_y x' y'], \quad (8)$$

and H'_0 is the Hamiltonian H_0 in the coordinate system (x', y', z') . We diagonalize the quadratic form $W'(x', y')$ by the rotation of the coordinate system around z' axis at the angle $\beta = (1/2) \arctan[2\omega_x \omega_y / (\omega_y^2 - \omega_x^2 + \Omega_x^2 - \Omega_y^2)]$ and obtain as a result

$$W''(x'', y'') = \frac{m^*}{2} (\lambda_1 x''^2 + \lambda_2 y''^2), \quad (9)$$

where λ_1, λ_2 are determined from the equation

$$\begin{vmatrix} \Omega_x^2 + \omega_y^2 - \lambda & -\omega_x \omega_y \\ -\omega_x \omega_y & \Omega_y^2 + \omega_x^2 - \lambda \end{vmatrix} = 0. \quad (10)$$

In the changed coordinate system (x'', y'', z') , the Hamiltonian H' reduces to the form

$$H'' = H''_0 + W'' + \frac{p_z^2}{2M}. \quad (11)$$

Since the parallel translations and rotation we used do not change the z component of the field \mathbf{B} , H''_0 is the Landau operator in the (x'', y'') plane with the magnetic field $B_z \mathbf{k}$. Therefore, the spectrum of $H''_0 + W''$ consists of the eigenvalues

$$\varepsilon_{mn} = \hbar \omega_1 (m + 1/2) + \hbar \omega_2 (n + 1/2), \quad (12)$$

where the hybrid frequencies ω_1, ω_2 have the form^{25,26}

$$\omega_{1,2} = \frac{1}{2} \{ [\Omega_x^2 + \Omega_y^2 + \omega_c^2 + 2\Omega_x \Omega_y \sqrt{1 + (\omega_x / \Omega_y)^2 + (\omega_y / \Omega_x)^2}]^{1/2} \pm [\Omega_x^2 + \Omega_y^2 + \omega_c^2 - 2\Omega_x \Omega_y \sqrt{1 + (\omega_x / \Omega_y)^2 + (\omega_y / \Omega_x)^2}]^{1/2} \}^{1/2} \quad (13)$$

(here $\omega_c = |e|B/m^*c$ is the cyclotron frequency).

Finally, for the spectrum of H , which is an invariant of unitary transformations, we have the expression

$$\varepsilon_{mnp_z} = \hbar \omega_1 (m + 1/2) + \hbar \omega_2 (n + 1/2) + p_z^2 / 2M. \quad (14)$$

III. BALLISTIC TRANSPORT IN THE QUANTUM WIRE

At the temperature $T=0$, the conductance of the quantum wire is described by the Landauer-Büttiker formula

$$\frac{G}{G_0} = \sum_{mm'nn'} T(m', n' \rightarrow m, n), \quad (15)$$

where $T(m', n' \rightarrow m, n)$ is the transition probability of the corresponding mode through the wire. Since in the case of the ballistic transport the quantum numbers m and n are not changed, then

$$T(m', n' \rightarrow m, n) = \delta_{m'm} \delta_{n'n}. \quad (16)$$

As a result, we can obtain from Eq. (15)

$$\frac{G(\varepsilon, B)}{G_0} = \sum_{n=0}^N \left[\frac{\omega_1}{\omega_2} (n + \delta) \right] + N + 1. \quad (17)$$

where N and δ denote the integer and fractional part of the number $(2\varepsilon - \hbar \omega_1 - \hbar \omega_2) / 2\hbar \omega_1$, respectively, ε is the energy of the particle, and the square brackets in Eq. (17) denote the integer part of a number. When the frequencies are incommensurable, the conductance undergoes the jumps with the change of N , when N changes to one unit. The jump is equal to the quantum of the conductance G_0 . Note that N depends on the energy of the particle and on the magnitude and the direction of the field \mathbf{B} . Hence, the conductance steps arise not only on the curve $G(\varepsilon)$ but also on the curve $G(\mathbf{B})$ both with the change of the magnitude and the direction of the field \mathbf{B} . The orientation of the field with respect to the coordinate system (x, y, z) is determined by an azimuthal angle θ and polar angle φ . Therefore, it is clear that the conductance steps arise both on the curve $G(\theta)$ and $G(\varphi)$ [see Eqs. (13) and (17)]. The plot of the dependences $G(\varepsilon)$, $G(B)$, $G(\theta)$, and $G(\varphi)$ are shown in Figs. 1 and 2 (the solid line). To analyze in detail the effect of temperature on the conductance, the following observation is very useful. For two-dimensional gas of the oscillators with the frequencies ω_1, ω_2 , the number of states $\nu(\varepsilon)$ with the energy less or equal to ε is equal to the number of the conductance quantum G/G_0 [this follows from Eq. (17)]. The classical partition function Z for this gas has the form²⁷

$$Z^{-1} = 4 \sinh\left(\frac{\hbar \omega_1}{2T}\right) \sinh\left(\frac{\hbar \omega_2}{2T}\right). \quad (18)$$

Using a formula that is similar to formula (11) from Ref. 27, we can express a number of states $\nu(\varepsilon)$ in terms of the classical partition function Z ,

$$\nu(\varepsilon) = \frac{1}{2\pi i} \int_{\alpha - i\infty}^{\alpha + i\infty} Z(\zeta) e^{\varepsilon \zeta} \frac{d\zeta}{\zeta} \quad (19)$$

(here $\alpha > 0$, $\zeta = 1/T$). It follows that $\nu(\varepsilon)$ is determined by simple poles of the integrand, lying on the imaginary axis, and by a triple pole at zero. The poles on the imaginary axis are multiple, if $n\omega_1 = m\omega_2$ for some positive n and m , and are simple in the opposite case. Since a real number is irrational with the probability one, then we can restrict this to the case of incommensurable frequencies. Using the same contour as in Ref. 27 for the calculation $\nu(\varepsilon)$, we obtain after some algebra

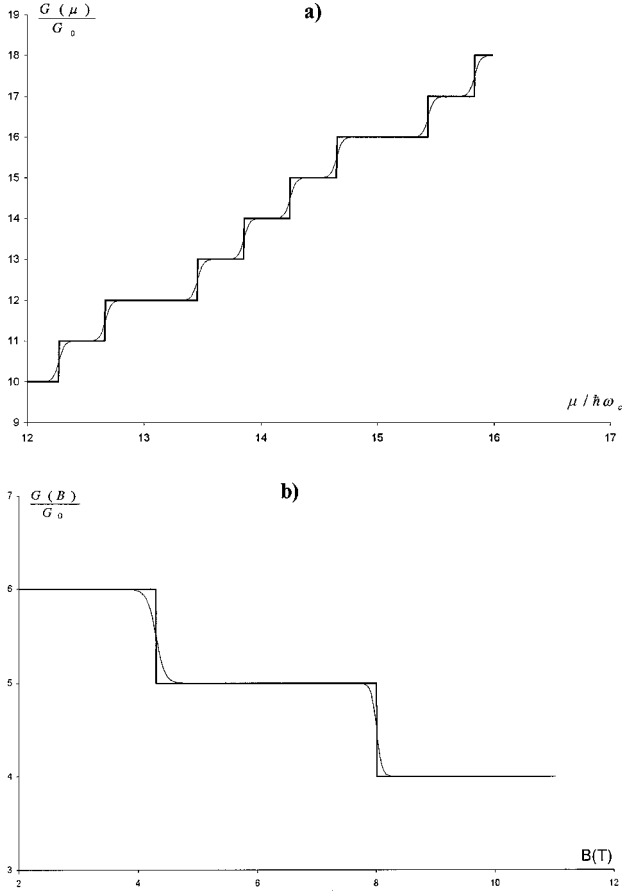


FIG. 1. (a) The conductance as a function of the chemical potential of the gas: $\Omega_x = 1.8 \times 10^{13} \text{ s}^{-1}$, $\Omega_y = 1.1 \times 10^{13} \text{ s}^{-1}$, $T = 1 \text{ K}$, $B = 2 \text{ T}$, $\theta = \pi/6$, $\phi = \pi/3$. (b) The conductance as a function of strength of the magnetic field B : $\Omega_x = 1.8 \times 10^{13} \text{ s}^{-1}$, $\Omega_y = 1.1 \times 10^{13} \text{ s}^{-1}$, $T = 1 \text{ K}$, $\mu/\hbar\sqrt{\Omega_x\Omega_y} = 3.3713$, $\theta = \pi/6$, $\phi = \pi/3$.

$$\begin{aligned} \frac{G(\varepsilon, 0)}{G_0} &= \frac{1}{2\hbar^2\omega_1\omega_2} \left(\varepsilon^2 - \frac{\hbar^2\omega_1^2 + \hbar^2\omega_2^2}{12} \right) \\ &+ \frac{1}{2\pi} \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \left[\frac{\cos(2\pi n\varepsilon/\hbar\omega_1)}{\sin(\pi n\omega_2/\omega_1)} \right. \\ &\left. + \frac{\cos(2\pi n\varepsilon/\hbar\omega_2)}{\sin(\pi n\omega_1/\omega_2)} \right]. \end{aligned} \quad (20)$$

The Fourier series in Eq. (20) originates from summation of the residues corresponding to the poles on the imaginary axis. The first term in this formula originates from the contribution of the pole at zero.

The formula (20) is more convenient for the study of the conductance than the starting expression (17). The first term in Eq. (20), which contributes to the monotone part of $G(\varepsilon)$, increases quadratically with ε . The Fourier series in Eq. (20) gives the oscillating part of the conductance. It is clear that each Fourier series depends on the fractional part $0 \leq \delta_j < 1$ ($j=1,2$) of the expression $\varepsilon/\hbar\omega_j$. Therefore, the first Fourier series as a function of ε has the period $\hbar\omega_1$, and the second one has the period $\hbar\omega_2$. The conductance steps are stipulated by the saw-toothed spikes in the oscillating part of $G(\varepsilon)$. Formula (20) is convenient for the determination of

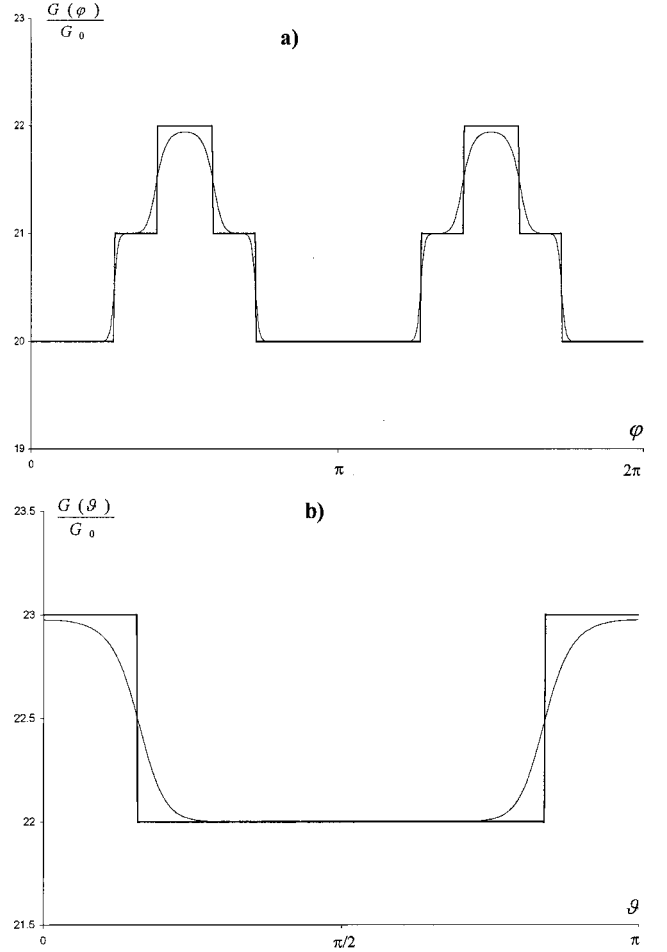


FIG. 2. (a) Plot of G as a function of angle ϕ : $\Omega_x = 1.8 \times 10^{13} \text{ s}^{-1}$, $\Omega_y = 1.1 \times 10^{13} \text{ s}^{-1}$, $T = 1 \text{ K}$, $B = 2 \text{ T}$, $\mu/\hbar\sqrt{\Omega_x\Omega_y} = 6.74259$, $\theta = \pi/6$. (b) Plot of G as a function of angle θ : $\Omega_x = 1.8 \times 10^{13} \text{ s}^{-1}$, $\Omega_y = 1.1 \times 10^{13} \text{ s}^{-1}$, $T = 1 \text{ K}$, $B = 1.7 \text{ T}$, $\mu/\hbar\sqrt{\Omega_x\Omega_y} = 6.74259$, $\phi = \pi/3$.

the temperature dependence of the conductance. From the formula

$$\frac{G(\mu, T)}{G_0} = \int_0^{\infty} G(\varepsilon, 0) \frac{\partial f}{\partial \mu} d\varepsilon, \quad (21)$$

where μ is the chemical potential of the electron gas in the wire, we obtain

$$\begin{aligned} \frac{G(\mu, T)}{G_0} &= \frac{1}{2\hbar^2\omega_1\omega_2} \left[2T^2 F_1\left(\frac{\mu}{T}\right) - \frac{1}{12} \hbar^2(\omega_1^2 + \omega_2^2) \right. \\ &\left. \times (1 + e^{-\mu/T})^{-1} \right] + \pi T \sum_{n=1}^{\infty} (-1)^{n+1} \\ &\times \left[\frac{1}{\hbar\omega_1} \frac{\cos(2\pi n\mu/\hbar\omega_1)}{\sinh(2\pi^2 nT/\hbar\omega_1) \sin(\pi n\omega_2/\omega_1)} \right. \\ &\left. + \frac{1}{\hbar\omega_2} \frac{\cos(2\pi n\mu/\hbar\omega_2)}{\sinh(2\pi^2 nT/\hbar\omega_2) \sin(\pi n\omega_1/\omega_2)} \right]. \end{aligned} \quad (22)$$

Here $F_1(\mu/T)$ is the Fermi integral. Suppose that $\mu \gg T$, then from Eq. (22) we get the estimation

$$\begin{aligned} \frac{G(\mu, T)}{G_0} = & \frac{1}{2\hbar^2\omega_1\omega_2} \left[\mu^2 + \frac{\pi^2 T^2}{3} - \frac{1}{12} \hbar^2 (\omega_1^2 + \omega_2^2) \right] \\ & + \pi T \sum_{n=1}^{\infty} (-1)^{n+1} \\ & \times \left[\frac{1}{\hbar\omega_1} \frac{\cos(2\pi n\mu/\hbar\omega_1)}{\sinh(2\pi^2 nT/\hbar\omega_1) \sin(\pi n\omega_2/\omega_1)} \right. \\ & \left. + \frac{1}{\hbar\omega_2} \frac{\cos(2\pi n\mu/\hbar\omega_2)}{\sinh(2\pi^2 nT/\hbar\omega_2) \sin(\pi n\omega_1/\omega_2)} \right]. \quad (23) \end{aligned}$$

Using Eq. (23), it is possible to estimate the ratio of the monotone part of the conductance to the oscillating one at $T \neq 0$:

$$\frac{G^{\text{osc}}}{G^{\text{mon}}} \sim \frac{T\hbar(\omega_1 + \omega_2)}{\mu^2}. \quad (24)$$

The dependences $G(\varepsilon)$, $G(B)$, $G(\theta)$, and $G(\varphi)$ at $T \neq 0$ are shown in Figs. 1 and 2 (the thin lines).

IV. DISCUSSION

As follows from the obtained results, the height of the conductance steps for the incommensurable frequencies is always equal to the conductance quantum G_0 . The width of a conductance plateau varies with the μ and the frequency ratio ω_1/ω_2 . The number of steps on an interval of variation of μ for fixed length of the interval depends on the position of the interval on the μ axis and on the frequency ratio ω_1/ω_2 . The behavior of the steps on the curves $G(B)$, $G(\theta)$, and $G(\varphi)$ is similar. Hence, relatively small change of the geometry of the system (namely, the variation of Ω_j , B , θ , or φ), which leads to the small variation of frequencies ω_j , can lead to the drastic change of the plot of the conductance $G(\mu)$. The reason for such sensitivity of the conductance to the geometry of the system can be seen from expression (18). Really, in the region where N is constant, the value $\omega_1\delta/\omega_2$ varies with the variation of ε , B , θ , or φ . This leads to variation of the magnitude of each term in Eq. (18). The effect of the temperature leads to a smearing of thresholds on

the steps of the conductance quantization and to an inclination of plateaus (Figs. 1 and 2). As pointed out earlier, the saw-tooth spikes arise on the conductance steps, these spikes are stipulated by the oscillating part of the conductance, namely, by the Fourier series in Eq. (22). The following circumstance stipulates such a form of the spikes. Since the amplitudes of harmonics in the series (20) decreases very slowly as n increases (namely, $\sim 1/n$), then a large number of terms of this series gives the contribution to the form of a spike. On the contrary, Eq. (23) shows that at $T \neq 0$ the contribution of higher harmonics is suppressed by factors $\sinh^{-1}(2\pi^2 nT/\hbar\omega_j)$. This leads to a substantial smearing of the saw-tooth spikes on the plot of G^{osc} even at relatively low temperature (~ 10 K). In turn, this effects the smearing of the step thresholds and the inclination of the plateaus on the plot of $G(\mu)$. In the case when the Fourier series has infinitely many members that are arbitrarily large, these members correspond to the indices n such that $n\omega_2/\omega_1$ or $n\omega_1/\omega_2$ are close to an integer. Hence, the summation of the series comes across the difficulties related to ‘‘small denominators problem.’’ The well-known Kolmogorov-Arnold-Moser theory overcomes these difficulties by restricting to the frequencies ω_1 and ω_2 , which satisfy the so-called Diophantine condition of incommensurability. The question of the convergency of the Fourier series in this case has been discussed in Ref. 27. If the wire has a circular cross section, $\Omega_x = \Omega_y = \Omega$, then Eq. (13) implies that

$$\begin{aligned} \omega_{1,2} = & \frac{1}{2} \{ [\omega_c^2 + 2\Omega^2 + 2\Omega\sqrt{\Omega^2 + \omega_c^2 - \omega_z^2}]^{1/2} \\ & \pm [\omega_c^2 + 2\Omega^2 - 2\Omega\sqrt{\Omega^2 + \omega_c^2 - \omega_z^2}]^{1/2} \}^{1/2}. \quad (25) \end{aligned}$$

In this case the frequencies ω_j are independent of the angle θ , and hence, the dependence of the conductance on this angle disappears. Therefore, the dependence of the conductance on the angle θ is a test of the deviation of the cross section from the circular form.

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