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On quantized electrical conductance

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Abstract

The quanta of electrical conductance is derived for a one-dimensional electron gas both by making use of the quasi-classical motion of a quantum fluid and by using arguments related to the uncertainty principle. The result is extended to a nanowire of finite cross-section area and to electrons in magnetic field, and the quantization of the electrical conductance is shown.

Recently, there is a considerable deal of interest in the quantized electrical conductance of atomic and molecular conductors like nanowires, narrow atomic constrictions, quantum dots, carbon nanotubes, etc.[1]-[11] The effect was originally predicted by Landauer.[12]-[14] We present here a new derivation of the quanta of electrical conductance for a one-dimensional electron gas, by making use of two procedures: the quasi-classical approach to the one-dimensional quantum electron fluid and by using arguments related to the uncertainty principle. We extend the results to the quantization of the electrical conductance in a quasi one-dimensional nanowire of finite area of the cross-section, where the electron motion is confined to the transversal direction while the free longitudinal motion is subjected to the action of the electric field. We apply also the present approach to electrons in a magnetic field.

We consider first a purely one-dimensional (free) electron gas in a conductor of length l and cross-section area A. We consider a purely quantum transport in such a conductor, without scattering or thermal effects. The electron density is given by $n = gk_F/\pi A$, where k_F is the Fermi wavevector and g is a degeneracy factor (*e.g.* $g = 2$ for spin 1/2). In the presence of an electric field E along the conductor the density is modified at the Fermi level by δn, such that, locally, higher energy levels are occupied for the electrons moving oppositely the field and Fermi energy levels are depleted for electrons moving along the field. We take the field oriented along the negative x-direction, so the net flow of electrons takes place along the positive x-direction. The electric field is sufficiently weak and slowly varying such that the electrons acquire a displacement $u(x)$ which obeys the quasi-classical equation of motion $m\ddot{u} = eE$, where m is the electron mass and $-e$ is the electron charge. The change in the electron density is given by $\delta n = -n\partial u/\partial x$, such that the density of electrons participating in the electrical flow is $-\delta n$. From these two equations we get straightforwardly

$$m\frac{d}{dt}\delta n = -enE/v_F \tag{1}$$

for a constant field, where v_F is the Fermi velocity. This is the basic equation for computing the electrical current.[1] Indeed, the electrical flow (charge per unit area of the cross-section and per unit

[1]The quasi-classsical motion of the one-dimensional quantum electron gas was previously discussed in more detail in Ref. 15.

time) is given by $j = -e(-\dot{\delta n})l = -e^2 nEl/mv_F$, hence the well-known electrical conductivity $\sigma = e^2 nl/mv_F$. The electrical flow is negative, *i.e.* it is oriented along the electrical field as it should be. For the one-dimensional gas $n = gk_F/\pi A$ and $v_F = \hbar k_F/m$, so we get $\sigma = g(2e^2/h)(l/A)$, where h is Planck's constant ($\hbar = h/2\pi$). The electrical conductance is $G = \sigma A/l = g(2e^2/h)$. We can see that the electrical conductance is quantized in units $G_0 = 2e^2/h$, according to the degeneration factor g.

It is worth noting that the same result can be obtained by applying the uncertainty principle. Indeed, the equation of motion $md\dot{u}/dt = eE$ can also be written as $m\dot{u} = eE\tau$, where τ is the time of motion. The electrical flow can be written as $j = -e\dot{u}\delta n$, where $\delta n = g\delta k_F/\pi A$ is the density of electrons participating in conduction. Combining these two equations we get $j = -e^2 E\tau\delta n/m$ and $\sigma = e^2\tau\delta n/m = ge^2\tau\delta k_F/\pi Am$, which is another representation for the electrical conductivity. Now, we use the uncertainty principle in the form $\tau = \delta n_F(h/\delta E)$, where $\delta n_F = l\delta k_F/2\pi$ and the change in energy is given by

$$\delta E = \frac{\hbar^2}{2m}(k_F + \delta k_F)^2 + \frac{\hbar^2}{2m}(k_F - \delta k_F)^2 - \frac{\hbar^2}{m}k_F^2 = \frac{\hbar^2}{m}(\delta k_F)^2 \ . \tag{2}$$

The motion time given by the uncertainty principle corresponds to δn_F cycles of quanta of action h. The change in energy given by (2) is also $\delta E = -eV$, where V is the voltage drop, which shows that the voltage is also quantized. We consider the energy levels sufficiently dense as to allow a continuous change in the electrical potential. Combining all these formula given above we arrive again at the conductance $G = gG_0$.

Within the quasi-classical description by means of the displacement field u the electrical field is given by $E = d\varphi/du$, where φ is the electrical potential, such that the equation of motion $m\ddot{u} = eE$ ensures the conservation of energy. This equation of motion can also be written as $\dot{\Pi} = eE = ed\varphi/du$, or $\dot{u} = ed\varphi/d\Pi$, where $\Pi = m\dot{u}$ is the momentum associated to the field u. One may check indeed that $\Pi = \hbar\delta k_F$ by making use of equation (2), so we may also write $\dot{u} = ed\varphi/dp = ed\varphi/\hbar dk_F$. Now, the electrical flow $j = -e\dot{u}\delta n$ becomes $j = -e^2(d\varphi/\hbar dk_F)\delta n = -e^2(dn/\hbar dk_F)V$ (since $\delta n = (dn/d\varphi)V$), hence the electrical current $I = jA = -gG_0V$. This was, in essence, the original argument of Landauer.[14] One can see that the conductance is proportional to the density of states.[2]

We consider next a nanowire of thickness d ($A = d^2$) and a confined transversal motion of the electrons, such that the energy levels are given by

$$E = \frac{\hbar^2 k^2}{2m} + \frac{\pi^2\hbar^2}{2md^2}(n_1^2 + n_2^2) \ , \tag{3}$$

where $n_{1,2}$ are positive integers.[3] We have now multiple branches of one-dimensional electron gas and the Fermi wavevector depends on the duplex (n_1, n_2). Therefore, the electron density is given by

$$n = (g/\pi A)\sum_{(n_1,n_2)} k_F(n_1, n_2) \tag{4}$$

and the electrical conductivity $\sigma = e^2 nl/mv_F$ becomes now

$$\sigma = (ge^2 l/\pi Am)\sum_{(n_1,n_2)} k_F(n_1, n_2)/v_F(n_1, n_2) \ . \tag{5}$$

[2] See in this respect Ref. 3.

[3] We impose fixed-ends boundary conditions for the transversal motion as for electrons confined in a potential well (see Refs. 1-3).

By equation (3), the Fermi velocity is $v_F = \hbar k_F/m$, such that the above electrical conductivity becomes $\sigma = gG_0(l/A)M$ and the electrical conductance is quantized according to $G = gG_0M$, where

$$M = \sum_{(n_1,n_2)} 1 \tag{6}$$

is the number of branches in the electron spectrum (number of channels).

Now we want to compute the number of channels M for this model. We assume a dense distribution of spectrum branches and write $n_1^2 + n_2^2 = \rho^2$ in equation (3). The chemical potential μ is established by the equalities

$$\mu = \frac{\hbar^2 k_F^2}{2m} + \frac{\pi^2\hbar^2}{2md^2}\rho^2 \ , \tag{7}$$

hence the Fermi wavevector k_F which is used in equation (4). The number of channels is then given by $M = \pi N_t^2$, where N_t is the highest integer ρ satisfying equation (7). It is given approximately by $N_t^2 = 2md^2\mu/\pi^2\hbar^2$. Equation (4) can then be written as

$$n = (2g/A)\int_0^{N_t} d\rho \cdot \rho\sqrt{2m\mu/\hbar^2 - \pi^2\rho^2/d^2} \ . \tag{8}$$

This equation gives a relationship between N_t and μ, which, together with the equation $N_t^2 = 2md^2\mu/\pi^2\hbar^2$ written above, serves to determine both the chemical potential μ and the number N_t of transverse channels, hence the number total of channels M, as a function of the density of the electron gas. The integral in equation (8) can be performed straightforwardly. We get $N_t = (3N/2\pi g)^{1/3}$ and $M = \pi^{1/3}(3N/2g)^{2/3}$, where N is the total number of electrons. The electrical conductance reads $G = G_0(\pi g)^{1/3}(3N/2)^{2/3}$.

As it is well-known, for electrons in a magnetic field H we can write the energy levels as

$$E = \frac{\hbar^2 k^2}{2m} + \hbar\omega_c(n + 1/2) + \mu_B H\sigma \ , \tag{9}$$

where $\omega_c = eH/mc$ is the cyclotron frequency, $\mu_B = e\hbar/2mc$ is the Bohr magneton and $\sigma = \pm 1$. Equation (5) gives now $G = G_0M$, where

$$M = \sum_{n\sigma} 1 \ . \tag{10}$$

It is approximately $M = 2n_l$, which is in fact twice the number of spectrum branches. We have also $\mu = \hbar\omega_c n_l$, where μ is the chemical potential given by

$$n = \frac{4eH}{\pi ch}\int_0^{n_l} \sqrt{2m\mu/\hbar^2 - 2m\omega_c n/\hbar} \ , \tag{11}$$

which is similar with equation (8). Here it is worth noting the well-known transversal degeneracy $2eHA/ch$ ($\gg 1$) of the energy levels in the magnetic field. We get $M = (3\sqrt{\pi}/4\sqrt{2})^{2/3}n^{2/3}ch/eH$ (which should be much larger than unity). It is worth emphasizing that the electrical conductance (or magnetoresistance) can be varied in quantum steps by varying the magnetic field, as it is well-known.

The inclusion in such a treatment of interaction, scattering or thermal effects (or finite-size boundary effects), as well as other particularities,[4] renders the problem a bit more complicated. Generally speaking, the starting point in such a treatment is the notion of elementary excitations and their lifetime. Particularly interesting is this problem for multi-wall carbon nanotubes, due to their specific electron energy structure.[6]

[4] *e.g.* for specular reflection in a cylindrical conductor in magnetic field see Ref. 8.

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