Quantum Conductance and Electrical Resistivity^{*}

P. R. SILVA, *CLÁUDIO NASSIF, MARCOS SAMPAIO AND M. C. NEMES

*Centro Brasileiro de Pesquisas Físicas-CBPF Rua Dr. Xavier Sigaud 150 22290-180, Rio de Janeiro, RJ

Departamento de Física - ICEx - UFMG Caixa Postal 702 30.123-970 - Belo Horizonte - MG - Brazil

cnassifCBPF@yahoo.com.br, prsilva@fisica.ufmg.br carolina@fisica.ufmg.br

January 17, 2007

Abstract

The Landauer formula for quantum conductance, based on the modern paradigm: "conduction is transmission", is generalized to samples of macroscopic size. Two regimes of electrical conduction, namely diffusive and ballistic ones, are studied. In the former regime, Drude's formula for the electrical resistivity is recovered and it is found a maximum conductivity equal to $(e^2mc)/(\pi\hbar^2)$, which is of the same order of magnitude as that of good metals at room temperature. In the latter, it is obtained in three dimensions a quantum conductance which is compatible with the one deduced by Sharvin in the ballistic regime. It is also found in this case an electrical conductivity which depends on the size of the sample, in agreement with that measured in very pure metals at the temperature of liquid helium. In two dimensions, the result for the conductance in the ballistic regime is consistent with that used to analyse quantum point contacts.

PACS numbers: 11.15.Tk

1 Introduction

A conventional view of the electrical conductivity attributes the onset of it to the linear response of the free electrons to the applied external electric field. This picture is contemplated both in classical Drude-Sommerfeld-Lorentz and in the quantum mechanical Kubo treatments. On the other hand, a modern view of the electrical conductance was proposed by Landauer [1], [2], which states that conduction is transmission (see also [3]). Both the conventional and modern views are treated in a paper by Rammer [4] in which, among other relevant considerations, discusses the connection between linear response formalism and the Landauer approach by expressing the conductance in terms of scattering properties of the sample. A microscopic viewpoint of electrical conductance based on kinetic theory and the role of local conservation laws is discussed in [20].

As pointed out by Batra in [5], it is well known that for an ideal one dimensional conductor under ballistic transport conditions, the conductance is transversely quantized in steps of $2e^2/h$ as the constriction width is varied. According to Batra [5], [6], the finite resistance of a perfect conductor, which has been previously understood in terms of contact effects, can also be viewed as having quantum mechanical origin in the uncertainty principle.

Landauer [1], [2] obtained a relation of the conductance for a one dimensional sample connecting two reservoirs at different electrochemical potentials through ideal conductors. In the absence of dissipative scattering the conductance G is given by

$$G = \frac{e^2}{\pi\hbar}T,\tag{1}$$

where T is the transmission probability of the sample, e the quantum of electrical charge and \hbar the reduced Planck's constant.

In the particular case where we have N perfectly transmitting channels, the conductance becomes

$$G = \frac{e^2}{\pi\hbar}N.$$
 (2)

Experimental verification of equation (2) comes from the study of quantum point contacts (QPC) [7], [8]. In a two dimensional heterojunction the channel width can be controlled by external applied gate voltages. The

^{*}Physics Letters A, Volume 358, Issues 5-6, pp. 327-498 (30 October 2006)

conducting channel works approximately as a waveguide. As it is widened, the number of transverse eigenstates below the Fermi level increases. Then conductance steps corresponding to different values of N in equation (2), are observed [2], [3], [7], [8].

In this letter we aim to extend the validity of equation (2) to the case of macroscopic samples in any spatial dimension, once the number N of conducting channels is properly interpreted. We intend to make connections of relation (2) with the conduction of electricity in good metals at the room temperature, as well with very high impurity-free samples at very low temperatures. We will see that in the first case it is possible to deduce the Drude formula starting from the Landauer relation for te quantum conductance and also to estimate the "real" conductivity of a good metal in room temperature. In the second case we will obtain an electrical conductivity which depends on the size of the sample. We will see that our results compare with those obtained by Sharvin [9] and by Lifshits and Kaganov [10], [11]. Finally the ballistic regime will be treated from the point of view of a drag force induced by a turbulent flow.

2 The diffusion regime

As a starting point of this work let us take a hypercubic sample of a good conductor of size L. By considering that the free electrons which are able to participate in the electric conduction are those close to the Fermi level with momentum p_F , it is convenient to write the following action in momentum space

$$A_{deff} = \int_{(\Delta p)^d} \left(|\vec{\nabla}_p \psi|^2 - \frac{|\psi|^2}{2mE} \right) d^d \vec{p},\tag{3}$$

where Δp is the wavepacket width around $\vec{p_F}$, m is the electron mass, E the energy and d is the space dimension.

Thompson[12] has introduced a heuristic method (of the dimensions) as a tool to deal with the critical behavior of a system undergoing a second order phase transition † . One of the basic hypothesis of Thompson is that each term of the Landau-Ginzburg-Wilson free energy used to describe the cooperative system is separately scaled to be of the order of the unity. In what follows we extend this framework to the action given by equation (3). Now if each term of the action (3) is separately taken to be of order of the unity, we may substitute equality between integrals with equality between integrands

$$\vec{\nabla}_p \psi = \pm \frac{i}{\sqrt{2mE}} \psi. \tag{4}$$

A solution of equation (4) gives

$$\psi = \psi_0 e^{\pm \frac{i}{\sqrt{2mE}}p}.$$
(5)

It is possible based on (5) to construct a wavepacket centered on p_F . From the first term in the action (3), by using Thompson's prescription we may also write

$$\int_{(\Delta p)^d} |\vec{\nabla}_p \psi|^2 \, d^d \vec{p} \sim |\psi|^2_{av} (\Delta p)^{d-2} \sim 1.$$
(6)

Equation (6) implies that

$$|\psi|_{av}^2 \sim (\Delta p)^{2-d},\tag{7}$$

where "av" stands for the averaged quantity. Taking into account the uncertainty relations, namely $\Delta pL \sim \hbar$, enables us to write equation (7) as

$$|\psi|_{av}^2 \sim L^{d-2}.\tag{8}$$

On the other hand, it is possible to think the transmition as occuring through N linearly independent channels and we write

$$|\psi\rangle = \sum_{i=1}^{N} |i\rangle.$$
(9)

Relation (9) implies that

[†]For applications of Thompson's method see [13]

$$\langle \psi | \psi \rangle = N \propto \left| \psi \right|_{av}^2. \tag{10}$$

Therefore combining equations (2) and (10) we obtain

$$G(L) = \frac{e^2}{\pi\hbar} \left(\frac{L}{l_0}\right)^{d-2},\tag{11}$$

where l_0 is the size of a typical channel.

In their work about the scaling theory of the localization, Abrahams et al [14] have defined a generalized dimensionless conductance that they called "Thouless number" as

$$g(L) = \frac{G(L)}{e^2/2\hbar}.$$
(12)

Therefore we can identify $(L/l_0)^{d-2}$ as the "Thouless number" in the delocalized diffusive regime. The case d = 3 deserves a special attention. Thus from equation (11) we have in three dimensions

$$G_{d=3} = \left(\frac{e^2}{\pi\hbar l_0}\right)L.$$
(13)

On the other hand, for large g, macroscopic transport theory is correct and gives [14]

$$G(L) = \sigma L^{d-2},\tag{14}$$

where σ is the electric conductivity. Comparing (14) with (11) we get, in the three dimensional case,

$$\sigma = \frac{e^2}{\pi\hbar} \frac{1}{l_0},\tag{15}$$

where l_0 can be evaluated through the following reasoning. Suppose that we have *n* scatterers per unity of volume and let us consider a cylinder shaped tube with longitudinal size equal to the electron mean free path λ and radius equal to the geometric average of l_0 and ℓ_F , where $\ell_F = l_F/(2\pi)$ is the reduced Fermi wavelength. It must be stressed that *n* is numerically equal to the number of electrons per unity of volume, if we consider that electric conductivity always happens in a regime of charge neutrality. We write

$$n\pi l_0 \ell_F \lambda = 1. \tag{16}$$

Inserting l_0 given by (16) into (15) allows us to obtain

$$\sigma = \frac{e^2 n\lambda}{mv_F},\tag{17}$$

where v_F is the Fermi velocity of the charge carrier. Equation (17) is just the Drude formula for the electrical conductivity, but here it was deduced starting from an expression describing quantum conductance.

It is also worthwhile noticing that if l_0 is considered as the width of the transmission channel then there should be a lower bound for it, namely the reduced Compton wavelength of the electron. Inserting $l_0 = \hbar/(mc)$ in (15) yields

$$\sigma_{max} = \frac{e^2 mc}{\pi \hbar^2},\tag{18}$$

where σ_{max} means the maximum conductivity in the diffusive regime. It is interesting to observe that σ_{max} depends on universal constants. A numerical evaluation of (18) gives $\sigma_{max} \sim 10^8 (\Omega \cdot m)^{-1}$. Indeed electrical conductivities of this order of magnitude are typical of those measured in good metals at room temperature.

Another evaluation of the electrical resistivity of metals was accomplished by Lifshits and Kaganov [10], [11] (see also Brandt and Chudinov [15]). The result obtained by Lifshits and Kaganov (LK) is

$$\sigma_{LK} = \frac{2}{3}e^2 \frac{S_F \lambda}{(2\pi\hbar)^3} = \frac{4}{3} \frac{e^2}{\hbar} \frac{\lambda}{l_F^2},\tag{19}$$

where $S_F = 4\pi p_F^2$ and λ is the electron mean free path. Comparing (19) with (15) yields

$$\lambda = \frac{3}{4\pi} \frac{l_F^2}{l_0}.\tag{20}$$

If we consider as before that the size of the transmission channel is limited by the electron reduced Compton wavelength, we will have in the diffusive regime an upper bound to the electron mean free path given by

$$\lambda_{max} = \frac{3}{4\pi} \frac{mc \, l_F^2}{\hbar} \tag{21}$$

3 The Ballistic Regime

To analyse the ballistic regime, it is convenient to write the action

$$A_{ball} = \int_{(\Delta p)^d} \psi^* (\vec{\nabla}_p \psi - \frac{i\psi}{\sqrt{2mE}}) d^d \vec{p}.$$
 (22)

We can repeat steps which go from (6) to (11), by using Thompson's prescription applied to the first term of the action (22). After doing this, we obtain

$$G = \frac{e^2}{\pi\hbar} \left(\frac{L}{l_0}\right)^{d-1}.$$
(23)

It would be interesting to make a detailed investigation of (23) in the special cases of two and three spatial dimensions (d = 2 and d = 3). If we make the natural choice of identifying in (23) l_0 with l_F (the Fermi wavelength), we get in three dimensions

$$G(d=3)_{ball} = \frac{e^2}{\pi\hbar} \left(\frac{L}{l_F}\right)^2.$$
(24)

This result recovers the ballistic transport treatment introduced by Sharvin [9] (see also Brandbyge et al [16]).

By comparing (24) with relation (14) in the case d = 3, enables us to write

$$\sigma_{d=3} = \frac{e^2}{\pi\hbar} \frac{L}{l_F^2}.$$
(25)

We observe that in the case of very pure metallic crystals at the liquid helium or lower temperatures, the electrical conductivity depends on the size of the sample. According to C. Kittel [17], mean free paths as long as 10 cm have been observed in very pure metals in the liquid helium temperature range. It seems that in this case, the mean free path is ultimately determined by the size of the sample. Taking L = 10 cm and l_F as the Fermi wavelength of the copper, we get a electrical conductivity of the order of magnitude $10^{14} (\Omega .m)^{-1}$.

Now let us analyse the two dimensional case in the ballistic regime. From equation (23) we have

$$G(d=2)_{ball} = \frac{e^2}{\pi\hbar} \left(\frac{L}{l_F}\right).$$
(26)

When the measurement is done at very low temperatures in a very pure two dimensional macroscopic sample, the quantization of the conductance cannot be detected since we have in this case $L \gg l_F$. However, measurements in Ga As-Al Ga As heterojunctions show that each new channel of transmission is activated only when the width w increases as $\Delta w \equiv \Delta L = l_F$. This characterizes the onset of the quantum conductance as it can be seen in the work by van Houten and Beenakker[3](please see also [7] and [8]).

4 An Alternative View of the Ballistic Regime

A macroscopic body moving at speeds high enough so that the flow of air behind it is turbulent, is subject to a drag force D given by (see for instance Halliday and Resnick[18])

$$D = \frac{1}{2}C\rho Av^2.$$
(27)

Here A is the effective cross-sectional area of the body, ρ is the density of the fluid, v is the speed of the body and C a dimensionless coefficient.

We think that in the ballistic regime the electrical resistance of a good conductor can be represented by the collisions of the charge carriers with walls which have the size of the sample, so that the area of the walls are L^2 . We observe that the ultimate wall is that which separates the sample from the surrounding dielectric medium. Changing the reference frame, we can imagine a wall being draged by the "fluid" composed by the free electron gas. With these ideas in mind, we can suppose that the power dissipation P is given by

$$P = Dv_F = \frac{1}{2}C\rho Av_F^3,\tag{28}$$

where $\rho = nm$, n and m being respectively the number density and mass of charge carriers. Now impose the equality between the drag power (equation (28)) and the power dissipation due to Joule effect, namely,

$$P_J = GV^2, (29)$$

where G is the electrical conductance and V is the applied potential difference. Using n given by equation (16) and considering the equality between the powers given by (28) and (29), we can write

$$\frac{Cm^2 v_F^4 A}{h l_0 \lambda} = GV^2. \tag{30}$$

Finally using that

$$\frac{1}{2}mv_F^2 = eV, (31)$$

we obtain

$$G = \frac{2e^2}{h} \left(\frac{L^2}{l_0\lambda}\right),\tag{32}$$

where we have fixed C = 1/2 and $A = L^2$.

This result which has been deduced especifically for the three dimensional case can be easily extended to other dimensions reproducing the general result for the ballistic regime as displayed in equation (23).

5 Rectangular and non-cubic geometries

It would be interesting to extend the results obtained in sections 2 and 3 to the case of rectangular and non-cubic symmetries. Let us choose the z-axis as the direction that the electrical current is injected into the sample. First let us consider the diffusion regime in three dimensions. Applying Thompson's prescription to the first term of action (3), we have

$$\int \left|\vec{\nabla}_p \psi\right|^2 d^d \vec{p} \sim \left|\psi\right|^2_{av,diff} \left[\frac{\Delta p_x \Delta p_y \Delta p_z}{(\Delta p_z)^2}\right] \sim 1.$$
(33)

Taking into account the uncertainty principle, we write:

$$\Delta p_x L_x = \Delta p_y L_y = \Delta p_z L_z = \hbar, \tag{34}$$

which leads to

$$|\psi|_{av,diff}^2 \sim \frac{L_x L_y}{L_z}.$$
(35)

In a similar way we have proceeded for the symmetric case, we obtain

$$G_{diff} = \frac{e^2}{\pi\hbar} \left(\frac{L_x L_y}{L_z}\right). \tag{36}$$

Writting

$$G_{diff} = \sigma(\frac{L_x L_y}{L_z}),\tag{37}$$

we recover for the electrical conductivity σ the result displayed in (15).

Turnning out the ballistic regime, we start by considering three dimensional case. Applying Thompson's recipe to the first term of the action (22), we have

$$\int \left|\psi^* \vec{\nabla}_p \psi\right| d^d \vec{p} \sim \left|\psi\right|^2_{av, ball(d=3)} \frac{\Delta p_x \Delta p_y \Delta p_z}{\Delta p_z} \sim 1,\tag{38}$$

and by using (34), we get

$$|\psi|^2_{av,ball(d=3)} \sim L_x L_y. \tag{39}$$

Proceeding in analogous way we have done in the symmetric case we obtain

$$G_{ball}(d=3) = \frac{e^2}{\pi\hbar} (\frac{L_x L_y}{l_F^2}),$$
(40)

and by using (37) yields

$$\sigma = \frac{e^2}{\pi\hbar} \left(\frac{L_z}{l_F^2}\right). \tag{41}$$

Finally, for the ballistic regime in a rectangular geometry, we have

$$\int \left| \psi^* \vec{\nabla}_p \psi \right| d^d \vec{p} \sim \left| \psi \right|_{av, ball(d=2)}^2 \frac{\Delta p_x \Delta p_y}{\Delta p_z} \sim 1, \tag{42}$$

which after taking into account the uncertainty principle gives

$$\left|\psi\right|_{av,ball(d=2)}^{2} \sim L_{x},\tag{43}$$

and

$$G_{ball(d=2)} = \frac{e^2}{\pi\hbar} \left(\frac{L_x}{l_F}\right). \tag{44}$$

Naturally, all the old results obtained in the symmetric cases are recovered by setting $L_x = L_y = L_z = L$.

6 Concluding Remarks

It is interesting to remember that in the paper on the scaling theory of localization, Abrahams et al[14] have introduced the "Thouless number" (equation (12) of this paper). According to the present work it is possible to distinguish two classes of such quantity, one of them being $g_{diff} = (L/l_0)^{d-2}$, referring to the diffusive regime and the other $g_{ball} = (L/l_0)^{d-1}$ referring to the ballistic regime of the electrical conduction.

Finally it is worth to mention that both Landauer transport theory and Kubo's formula were used to compute DC conductance in a impurity system in a recent work by Castro-Alvaredo and Fring [19]. They found an identical plateau structure for the DC conductance in the ultraviolet limit, displaying the agreement between the two approaches.

References

- [1] R. Landauer, IBM J. Res. Dev. 1, 223 (1957); J. Phys. C 1, 8099 (1989).
- [2] Y. Imry and R. Landauer, Rev. Mod. Phys. 71, S 306 Centenary (1999).
- [3] M. Büttiker, Phys. Rev. B 35, 4123 (1987); H. van Houten and C. Beenakker, Phys. Today 49, 22 (July 1996).
- [4] J. Rammer, Rev. Mod. Phys. 63, 781, (1991).
- [5] I. P. Batra, Surf. Sci. **395**, 43 (1998).
- [6] I. P. Batra, Sol. State Comm. **124**, 463 (2002).

- [7] B. J. van Wees, H. van Houten, C. W. J. Beenakker, J. G. Williamson, L. P. Kouwenhoven, D. van der Marel, C. T. Foxon, Phys. Rev. Lett. 60, 848 (1988); Phys. Rev. B 43, 12431 (1991).
- [8] J. M. Krans, J. M. van Ruitenbeek, V. V. Fisun, I. K. Yanson, L. J. de Jongh, Nature 375, 767 (1995).
- [9] Yu. V. Sharvin, Sov. Phys. JETP **21**, 655 (1965).
- [10] I. M. Lifshits and M. I. Kaganov, Uspekhi Fiz. Nauk **69**, 419 (1969); Uspekhi Fiz. Nauk **78**, 411 (1962).
- [11] I. M. Lifshits, Sov. Phys. JETP 38, 1569 (1960).
- [12] C. J. Thompson, J. Phys. A 9, L25 (1976).
- [13] C. Nassif, P. R. Silva, Mod. Phys. Lett. B 13, 829 (1999); Mod. Phys. Lett. B 15, 33 (2001); Mod. Phys. Lett. B 15, 1205 (2001); Mod. Phys. Lett. B 16, 601 (2002); P. R. Silva, Phys. Stat. Sol. (b) 179, K5 (1993); Phys. Stat. Sol. (b) 165, K79 (1991); Phys. Stat. Sol. (b) 174, 497 (1992); Phys. Stat. Sol. (b) 179, K99 (1993); P. R. Silva and V. B. Kokshenev, Braz. J. Phys. 30, 783 (2000).
- [14] E. Abrahams, P. W. Anderson, D. C. Licciardello and T. V. Ramakrishnan, Phys. Rev. Lett. 42, 673 (1979).
- [15] N. B. Brandt and S. M. Chudinov, Electronic Structure of Metals, Mir Publishers, Moscow, 1975.
- [16] M. Brandbyge, J. Schiøtz, M. R. Sørensen, P. Stoltze, K. W.Jacobsen, J. K. Nørskov, L. Olesen, E. Laegsgaard, I. Stensgaard and F. Besenbacher, Phys. Rev. B 52, 8499 (1995).
- [17] C. Kittel, Introduction to Solid State Physics, Wiley, New York, 1976, p. 169.
- [18] D. Halliday, R. Resnick, Fundamentals of Physics, Third Edition Extended, Wiley, New York, 1988, p. 109.
- [19] O. Castro-Alvaredo, A. Fring, Nucl. Phys. B649, 449 (2003).
- [20] F. Green, M. Das, Transport, Noise, and Conservation in the Electron Gas: How to Build a Credible Mesoscopic Theory, cond-mat/0202426-v4.