Quantum size effect in thin-wire transport

Vijay K. Arora
Department of Physics, University of Riyadh, P.O. Box 2455, Riyadh, Saudi Arabia
(Received 27 May 1980; revised manuscript received 9 December 1980)

A quantum transport theory for electric conductivity is presented for the condition that the de Broglie wavelength of a thermal electron becomes comparable to the transverse dimensions of a thin wire of rectangular cross section. The theoretical results, which include the effect of size quantization, are analyzed in the ultrathin limit (UTL). In the UTL the ratio of longitudinal resistivity to bulk resistivity is shown to be proportional to λ_D^2/A, where λ_D is the de Broglie wavelength and A is the area of cross section. The results for transverse resistivity are also given and discussed.

In another paper[1] in this issue we have discussed the electronic transport in semiconductors limited to the size of a thin film. When the de Broglie wave-length λ_D of an electron is comparable to the dimensions of the sample, quantum effects become important and deviations from the bulk behavior in transport properties are expected. In contrast, the predictions of theories[2,3] based on the model of localization do exist. It has been shown that thin metal films or wires do not exhibit true metallic conductivity in the low-temperature limit. This and other predictions of the localization theories have been tested experimentally[4,5] and qualitative agreement obtained. A number of quantitative discrepancies remain, the most serious one being that of the temperature dependence.[4] In the following we study transport in thin wires of rectangular cross section by following the method of Ref. 1.

The Fermi energy ζ of a metal lies well above the conduction-band edge. But, when size quantization is taken into account, the lowest quantized energy $\epsilon_{z,y}$ (see below) of an electron may become larger than the Fermi energy. And, for a sufficiently thin sample, when $\epsilon_{z,y} \gg \zeta$, a metal may behave like a semiconductor. An analogous situation arises in transport properties of electrons confined to a strong magnetic field, when $\lambda_D \gg \lambda$, the radius of cyclotron orbit.[6] This behavior has not yet been tested in metals in a magnetic field, as the magnetic field required for this behavior appears to be quite large. But such behavior is becoming quite apparent in thin films and wires.

In a thin wire of rectangular cross section, the electronic motion in the transverse direction is quantized, with eigenfunctions ψ_{plk} and eigenvalues ϵ_{plk} given by

$$\psi_{plk} = (2/\Omega)^{1/2} \exp(ikx)\sin(p\pi y/b)\sin(l\pi z/d)\,, \quad p, l = 1, 2, 3 \tag{1}$$

$$\epsilon_{plk} = \hbar^2 k^2/2m^* + p^2\epsilon_y + l^2\epsilon_z\,, \tag{2}$$

with

$$\epsilon_y = \pi^2\hbar^2/2m^*b^2\,, \tag{3}$$

$$\epsilon_z = \pi^2\hbar^2/2m^*d^2\,, \tag{4}$$

where $\Omega = abd$ $(b, d \ll a)$ is the volume of the sample, k is the momentum of an electron parallel to the wire, and m^* is the effective mass of an electron. In the above, we have assumed the parabolic band structure of the material unaffected by the thinness of the wire.

The matrix elements of the components v_x, v_y, and v_z of the velocity vector in the representation of Eq. (1) are given by

$$\langle p'l'k'|\, v_x\,|plk\rangle = (\hbar k/m^*)\delta_{l'l}\delta_{p'p}\delta_{k'k}\,, \tag{5}$$

$$\langle p'l'k'|\, v_y\,|plk\rangle = 2\hbar pp'\{1 - \exp[i\pi(p'-p)]\}\delta_{l'l}\delta_{k'k}/im^*b(p'^2 - p^2) = 0 \quad \text{when } p = p'\,, \tag{6}$$

$$\langle p'l'k'|\, v_z\,|plk\rangle = 2\hbar ll'\{1 - \exp[i\pi(l'-l)]\}\delta'_{pp}\delta_{k'k}/im^*d(l'^2 - l^2) = 0 \quad \text{when } l = l'\,. \tag{7}$$

As is seen from Eqs. (5)–(7), the matrix elements of v_x are diagonal, while those of v_y and v_z are nondiagonal. This necessitates the use of the density matrix ρ for finding the expectation value of the current by following the procedure outlined in Ref. 1:

$$\langle \vec{j} \rangle = -\frac{e}{\Omega}\sum_{\alpha\alpha'} \langle \alpha'|\,\rho\,|\alpha\rangle\langle\alpha|\,\vec{v}\,|\alpha'\rangle\,, \tag{8}$$

where $\langle \alpha'|\,\rho\,|\alpha\rangle$ are given by

$$\langle \alpha'|\,\rho\,|\alpha\rangle = f_0(\epsilon_\alpha)\delta_{\alpha'\alpha} + \frac{\langle\alpha'|\,[\rho_0, F]\,|\alpha\rangle}{\epsilon_{\alpha'} - \epsilon_\alpha - i\hbar\tau^{-1}_{\alpha\alpha'}}\,, \tag{9}$$

with

$$\tau_\alpha^{-1} = \tau^{-1}(\epsilon_{plk}) = C\Big(\sum_{p'l'} (\epsilon_{plk} - p'^2\epsilon_y - l'^2\epsilon_z)^{-1/2} + \tfrac{1}{2}\sum_{p'} (\epsilon_{plk} - p'^2\epsilon_y - l^2\epsilon_z)^{-1/2} + \tfrac{1}{2}\sum_{l'} (\epsilon_{plk} - p^2\epsilon_y - l'^2\epsilon_z)^{-1/2} + \tfrac{1}{4}(\epsilon_{plk} - p^2\epsilon_y - l^2\epsilon_z)^{-1/2}\Big), \quad (10)$$

$$C = E_1^2 k_B T (2m^*)^{1/2}/bd\rho_d u^2\hbar^2 . \quad (11)$$

Here α stands for electron and lattice quantum numbers of the unperturbed system. E_1 is the deformation potential constant for acoustic-phonon scattering, k_B is the Boltzmann constant, T is the temperature, ρ_d is the material density of the wire, and u is the velocity of sound. Equation (10), which is written for acoustic-phonon scattering, also applies to point-defect scattering if $C = n_i V_0^2 (2m^*)^{1/2}/bd\hbar^2$ in Eq. (11), where n_i is the density of defects and V_0 is the potential parameter of the defect represented by a delta potential $V = V_0 \sum_i \delta(\vec{r} - \vec{r}_i)$. Using Eq. (8) and defining conductivity $\underline{\sigma}$ as $\langle \vec{j} \rangle = \underline{\sigma} \cdot \vec{\epsilon}$, the components of $\underline{\sigma}$, in the ultrathin limit, are obtained as

$$\sigma_{xx} = 8ne^2 \chi_D \hbar \rho_d u^2 A/9\sqrt{\pi} m^* E_1^2 , \quad (12)$$

$$\sigma_{yy} = (64ne^2\tau_0^{-1}\hbar^6/81 m^{*3} b^3 d\epsilon_y^3 k_B T) \times \exp\left(\frac{b\hbar/\tau_0}{2^{1/2}\pi^{3/2} d k_B T}\right)^2 E_1\left(\frac{b\hbar/\tau_0}{2^{1/2}\pi^{3/2} d k_B T}\right)^2 , \quad (13)$$

where n is the electronic density, $\chi_D = \hbar/(2m^* k_B T)^{1/2}$, A is the area of cross section of the wire, and

$$\tau_0^{-1} = 3(2m^* k_B T)^{3/2} E_1^2/8\pi^{1/2}\rho_d u^2 \hbar^4 , \quad (14)$$

$$E_1(\alpha) = \int_\alpha^\infty \frac{e^{-t}}{t}\, dt . \quad (15)$$

σ_{zz} can be obtained from the expression of σ_{yy} by interchanging b and d. When $\hbar\tau_0^{-1} \ll k_B T$, $Ei(\alpha) \approx -\ln\alpha - \gamma$ ($\alpha \ll 1$), where $\gamma = 0.577$ (Euler's constant), the relative resistivity ratios (as compared to bulk resistivity ρ_b) are given by

$$\rho_{xx}/\rho_b = 1/\sigma_{xx}\sigma_b = 4\pi\chi_D^2/3A , \quad (16)$$

$$\rho_{yy}/\rho_b = 1/\sigma_{yy}\sigma_b = (81 d\pi^6 k_B T/512\tau_0^{-2} b^3 m^*)\left[\ln\left(\frac{2^{1/2}\pi^{3/2} d k_B T}{b\hbar/\tau_0}\right) - \gamma\right]^{-1} , \quad (17)$$

where

$$\rho_b = 3(2\pi m^* k_B T)^{1/2} m^{*2} E_1^2 k_B T/4ne^2\rho_d u^2 \pi\hbar^4 . \quad (18)$$

Similar expression exists for ρ_{zz}/ρ_b by interchanging b and d in Eq. (17).

Although the above results are applicable to an idealized system of a rectangular wire, qualitatively the results should be applicable to wires of any general cross section. The longitudinal resistivity ratio is independent of the scattering parameters, is inversely proportional to area, and varies with temperature as T^{-1}. The absolute resistivity $\rho_{xx} \sim T^{+1/2}$ for acoustic-phonon scattering and $\rho_{xx} \sim T^{-1/2}$ for point-defect scattering. Since most of the thin-wire experiments are done at low temperature, it is highly unlikely that acoustic-phonon scattering plays a dominant role. At these low temperatures, point-defect scattering, which can be assumed to be dominant, gives temperature dependence consistent with the experimental results.[4] On the other hand, the localization theories give temperature dependence as $\rho_{xx} \sim T^{-2}$ which is highly inconsistent with the experimental data. The predictions of transverse resistivity ρ_{yy} and ρ_{zz} are probably quite difficult to test experimentally in the present state of technology. But, in the future, when such measurements are possible, Eq. (17) may be tested experimentally. Equation (17) also gives A^{-1} dependence for area for a wire of square cross section only. It may be noted that although the resistivity ratio ρ_{xx}/ρ_b is independent of scattering parameters, ρ_{yy}/ρ_b depends strongly on scattering parameters. With the developing technology for thin wires being produced by lithographic techniques, it is hoped that the above results will be useful in understanding the quantum character of an electron in confined systems.

The author wishes to thank his colleagues Dr. M. A. Al-Mass'ari and Dr. F. G. Awad for several stimulating discussions. He also wishes to acknowledge partial support from Faculty of Science Research Center of the University of Riyadh.

[1] V. K. Arora and F. G. Awad, this issue, Phys. Rev. B 23, 5570 (1981).
[2] D. J. Thouless, Phys. Rev. Lett. 39, 1167 (1977).
[3] E. Abrahams, P. W. Anderson, D. C. Licciardello, and T. V. Ramakrishanan, Phys. Rev. Lett. 42, 673 (1979).
[4] N. Giordano, W. Gilson, and D. E. Prober, Phys. Rev. Lett. 43, 725 (1979).
[5] G. J. Dolan and D. D. Osheroff, Phys. Rev. Lett. 43, 721 (1979).
[6] V. K. Arora, Phys. Status Solidi B 75, K65 (1976).