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Quantum-size effects in quasi-one-dimensional electrical conduction

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Abstract The diffusive and collisional contributions to the dc-electric current along a quantum wire, of width much smaller than the mean free path, are evaluated at very low temperatures for impurity scattering using a *quantum* Boltzmann equation. The electrons are assumed to be independent or to interact (binary collisions) in the presence of impurities. The lateral confinement is modelled with a square or a parabolic well and the vertical one by a triangular well. Due to the confinement the electronic motion becomes quasi-one-dimensional and changing the Fermi energy or the wire width leads to oscillations in the density of states, the scatteriug rate, and the conductivity. Level broadening is taken into account self-consistently.

Over the last years there has been a growing interest in systems of reduaed dimensionality such as quantum wires and quantum dots. When the width W of a two-dimensional electron gas becomes much smaller than the mean free path $l_e(\sim \mu m)$, the electronic motion becomes quasi-one-dimensional (Q1D). The quantum states become localized in the lateral direction and this leads to distinct quantized energy levels which modify the physical properties of the system. New quantum size-effects have been reported such as: non-local bend resistance[1], the quenching of the Hall effect[2], the oscillatory behavior of the capacitance[3] and of the conductivity[4], etc.

Previous studies of conduction in quantum wires have considered only the quantum size limit[5,6] or short-range impurity scattering[7] treating the lateral confinement with a square well; also, electron-electron interaction effects have been neglected, In this paper we present a more complete evaluation of the impurity limited conductivity in quantum wires: i) we model the lateral confinement both with a square and a parabolic potential well when an arbitrary number of conduction channels is occupied, and ii) we take into account, approximately, the effect of electron-electron interaction.

For the evaluation of the electrical conductivity, along the wire, we use general Kubo-type expressions derived, e.g. in ref.8, for weak scattering and weak electric fields. For one-body collisions the *diffusive* contribution σ_p to the dc conductivity is given by

$$\sigma_p = \frac{e^2}{\Omega} \sum_{\varsigma} \beta f_\varsigma (1 - f_\varsigma) v_\varsigma^x v_\varsigma^x \tau(E_\varsigma) \ , \tag{1}$$

and the ***collisional*** contribution by

$$\sigma_c = \frac{\beta e^2}{2\Omega} \sum_{\varsigma,\varsigma'} f_\varsigma (1 - f'_\varsigma) W_{\varsigma,\varsigma'} (X_\varsigma - X_{\varsigma'})^2 \ , \tag{2}$$

where $v_\varsigma^x = <\varsigma|\dot{x}|\varsigma>$ is the electron velocity in the x-direction associated with the state $|\varsigma>$ and $X_\varsigma = <\varsigma|x|\varsigma>$ its average position. $\tau(E_\varsigma)$ is the energy dependent relaxation time, $W_{\varsigma,\varsigma'}$ is the scattering rate and $f_\varsigma = <\mathrm{n}>_{eq}$ is the average occupancy of the state $|\varsigma>$ in the equilibrium situation. Further, Ω is the volume, $|e|$ the electron charge and $\beta = 1/k_B \mathrm{T}$. For transport through localizes states the diffusive contribution vanishes identically and there is only collisional current as in the case of hopping conduction and for transport in the quantum Hall regime .

For two-body collisions (e.g. electron-electron interaction) the diffusive contribution is approximately given by eq.(1) and the collisional one by[10]

$$\sigma'_c = \frac{\beta e^2}{4\Omega} \sum_{\varsigma_1,\varsigma_2,\varsigma_3,\varsigma_4} Q(\varsigma_1,\varsigma_2,\varsigma_3,\varsigma_4) f_{\varsigma_1} f_{\varsigma_2} (1 - f_{\varsigma_3})$$
$$(1 - f_{\varsigma_4})(X_{\varsigma_1} + X_{\varsigma_2} - X_{\varsigma_3} - X_{\varsigma_4})^2 \ , \tag{3}$$

where $Q(\varsigma_1, \varsigma_2, \varsigma_3, \varsigma_4)$ is the scattering rate of the transition $|\varsigma_1, \varsigma_2 > \rightarrow |\varsigma_3, \varsigma_4 >$.

The expressions (1)-(3) will be applied to a quantum wire of dimensions $L_x, L_y = W, L_z$, suchthat $L_y, L_z << l_e <<$ L, = L; W $\approx 0.1\mu m$ and L, $\approx 50 - 100\AA$. The confinement in the z-direction is rnodelled with a triangular well and it is assumed that only the lowest subband with energy E_z^0 is occupied. We model the lateral confinement with: 1) a ***square*** well of infinite depth and, **2)** a ***parabolic*** well of frequency w. The latter has been shown to be appropriate for very narrow wires[11]. The electrons are free along the x-direction. The main difference between the two models are: i) the harmonic oscillator potential gives an equidistant energy spectrum whereas a square well potential does not, ii) the wave function for a square well vanishes at y = 0 and y = W whereas that for a parabolic well does not, i.e. in the first case the confinement is rigid with a well-defined width, in the second case it is not. Both wave functions, however, are localized in the y-direction $(<\varsigma|v_y|\varsigma>= 0)$.

We model the elastic scattering of electrons by the quasi-one-dimensional random distribution of impurities with the potential

$$U(x) = U_0 \exp(-k_s|x)/\sqrt{|x|};$$

$$U_0 = 2\pi e^2\sqrt{c}/\epsilon,$$

with k_s the inverse screenning length, é the dielectric constant, and c a constant of order 1 in units of inverse length. The Fourier transform U_q of $U(x)$ is

$$U_q = U_0\sqrt{(k_s + \sqrt{q_x^2 + k_s^2})/(q_x^2 + k_s^2)}.$$

We will limit ourselves to the long-wavelength limit, $q_x \rightarrow 0$, $U_q^2 \rightarrow 2U_0^2/k_s$.

The unperturbed density of states $D(E)$ is proportional to

$$\sum_n 1/\sqrt{E - E_z^0 - E_n},$$

where E, $= n^2E_0$ for the square well and E, $= (n + \frac{1}{2})\hbar\omega$ for the parabolic one; it diverges for E $\rightarrow$ E, $+ E_z^0$. If we assume a Lorentzian broadening of the 6-function

with zero shift (equivalent to neglecting the real part of the Green's function) we obtain

$$D(E) = D_0 \sum_n S(\tilde{\epsilon}_n, \tilde{\Gamma}_n) \ , \tag{4}$$

where

$$S(\epsilon, \Gamma) = \sqrt{(\sqrt{\epsilon^2 + \Gamma^2} + \epsilon)/(\epsilon + \mathrm{r})} \ ,$$

with $D_0 = 2L\sqrt{m^*}/h\sqrt{E_0}$ and $E_0 = \hbar\omega$ for the parabolic well and $E_0 = \pi^2\hbar^2/2m^*\mathrm{W}^2$ for a square well. Further, $\tilde{\epsilon}_n = \epsilon_n/E_0$, $\tilde{\Gamma}_n = \Gamma_n/E_0$, with $\epsilon_n = \mathrm{E} - E_z^0 - \mathrm{E},$, and Γ_n is the level width. The divergence is now removed. Following ref.12 we find that we can neglect the real part of the Green's function and in this case $\Gamma_n(\mathrm{E}) \cong \Gamma_n$ is determined ***self-cnsistently*** by

$$\Gamma_n = (\hbar C'\sqrt{2}/4) \sum_{n'} B_{nn'} S(C_{n'}, \Gamma_{n'}) \ , \tag{5}$$

where

$$C' = (2N_I U_0^2 F/\hbar k_s)\sqrt{2m^*/\hbar^2}$$

and $C_{n'} = \mathrm{E} - E_{n'} - E_z^0 \cdot N_I$ is the impurity density $\sim 10^5 cm^{-1}$ and $B_{nn'}$ is a numerical factor resulting from $< \zeta' | e^{iq\cdot r} | \zeta >$ entering the evaluation of $W_{\zeta,\zeta'}$.

The DOS is evaluated by means of eqs.(5) and (4) for the square (fig.1a) and parabolic (fig.1b) wells for different values of the impurity scattering strength $\bar{\zeta} = \hbar C'\sqrt{2}/4E_0^{3/2}$. The DOS oscillates as a function of the energy: Also $\Gamma_n(\mathrm{E})$ exhbits oscillations which die out with increasing energy. It is apparent that increasing $\bar{\zeta}$ broadens the peaks in the DOS. A noticeable difference,however, occurs for high energies: for a square well the DOS oscillates around a constant value and looks more like the DOS of two-dimensional electron gas whereas for a parabolic well $D(E) \sim \sqrt{E}$ as in the case of a 3D system. In the former case the number of levels stays almost constant with increasing E (the level separation varies as .N^2). In the latter case the behavior of the DOS is a consequence of the softness of the potential: with increasing energy the potential becomes broadened and the electrons will be able to fill a larger area in space. Another noticeable feature of the DOS, common

to both confining potentials, is that there appears almost no difference for the result with $\Gamma =$ const. or with $\Gamma_n(\mathrm{E})$ as determined self-consistently except at the onset of the DOS. Therefore, in the following we take the level width constant and we have verified that this does not change our numerical results appreciably.

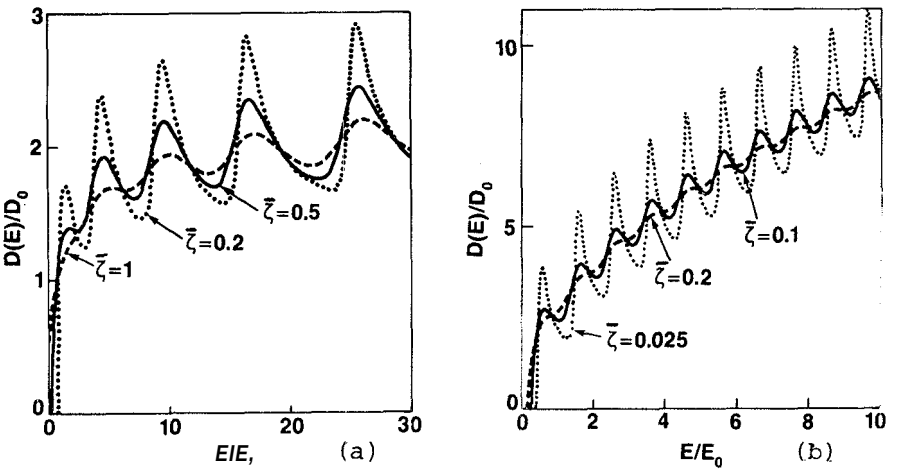

Fig.1 - Density of states (DOS) as function of the energy for different values of the electron-impurity interaction strength $\bar{\zeta} = 0.2, 0.5$ and 1. The confinement potentiai is a square well (fig. 1a) or a parabolic well (fig. 1b).

A. One-body collisions

The *diffusive* contribution is evaluated from eq.(1) with $\tau_n(\mathrm{E}) \approx \hbar/\Gamma_n(E)$. The result is

$$\sigma_p = \sigma_1 \sum_n \int_0^\infty dx \beta f_{nx}(1 - f_{nx}) x^2 \Big(\sum_{n'} B_{nn'} S(C_{nn'}, \Gamma_{n'}) \Big)^{-1}, \qquad (6)$$

where a, $= (8e^2/\sqrt{2}h)(\hbar^2 k_s/2m^*)/N_I U_0^2 F, C_{nn'} = x^2 + E_n - E_{n'}$, $x = \hbar k/\sqrt{2m^*}$, and $F = 9/16$.

The *collisional* contribution is evaluated with the approximation $X_\zeta - X_{\zeta'} \approx l_e$; we obtain

$$\sigma_c = \frac{\sigma_0}{\sqrt{2}} \sum_{n,n'} B_{nn'} \int_0^\infty dx \beta f_{nx}(1 - f_{nx}) S(C_{nn'}, \Gamma_{n'}) \quad , \tag{7}$$

where

$$\sigma_0 = (e^2/h)(2m^* l_e^2/\hbar^2)(N_I U_0^2 F/k_s).$$

The diffusive contribution σ_p, relevant for low impurity densities, as evaluated from eq.(6) shows the same dependence on the density (or Fermi energy) as that of ref. 7.

The collisional contribution a,, expressing hopping at high impurity densities, as evaluated numerically from eq. (7), is shown in fig. 2 for different temperatures ($\bar{\beta} = \beta E_0$) and fixed level width ($\bar{\Gamma} = \Gamma/E_0$) for a square well (fig. 2a) and a parabolic well (fig. 2b). Each time the Fermi energy passes through an energy level E,, the conductivity increases because a new conduction channel opens up. The difference the DOS of a square well and of a parabolic well also show up in the conductivity since the latter is just a convolution of the DOS with a combination of Fermi-Dirac functions expressing the occupancy of the states under consideration. Notice that the behavior of the conductivity is different from that in the ballistic regime. In this case the conductivity is quantized , a $\simeq n(2\epsilon^2/h)$, where n is the number of conducting channels. In the case under study the electron motion is considered over a distance L >> l_e such that many collisions have occurred between the two measuring probes. Because of the peak structure of the DOS the scattering rate will also be influenced and will reflect the structure in the DOS which will modulate the conductivity. This is clearly apparent in figs. 2a and 2b. This oscillatory structure has recently been observed[4] in a GaAs/AlGaAs quasi-one-dimensional FET. The dependence of the conductivity a, on the width of the wire is shown in fig. 3 for the square well potential. The solid curve is obtained upon keeping the 2D electron density $n_e^{2D} = n_e^{1D}/W$ constant (reminiscent of an isolated system) and the dashed curve is for a constant Fermi energy. The latter case corresponds physically to varying the width of the wire while keeping the system in electro-chemical contact with a bath of 2D or 3D electrons. In either

case: *1)* the conductivity increases with wire width W, and **2)** the conductivity oscillates with W in agreement with observations[4].

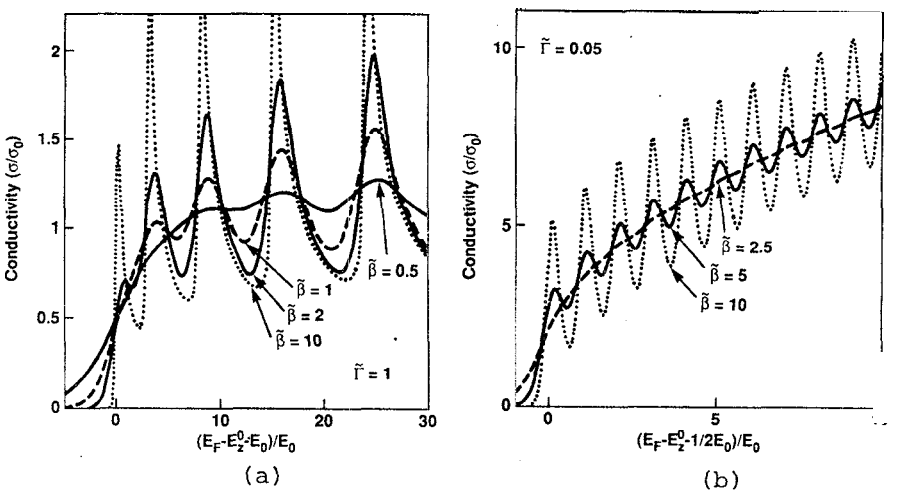

Fig.2 - The collisional contribution to the conductivity as a function of the Fermi energy (E_F) for different values of the inverse temperature $\tilde{\beta} = \beta E_0$ and fixed value of the level width $\tilde{\Gamma}$. The confining potential is a square well (fig.2a) or a parabolic well (fig.2b).

B. Two-body collisions

When the electrons interact, in the presence of impurities, the diffusion contribution is approximately given by eq.(1) and the collisional one by eq.(3), which is much more complicated than eq. *(2)*. To avoid excessive numerical work we limit ourselves to the square well in narrow wires where interlevel transitiuns are absent. We use the same model potential as before and make the approximation $X_{s_1} - X_{s_3} \approx X_{s_2} - X_{s_4} \backsim 1$,. The *6* function involved in the definition of $Q(...)$[8] becomes $\delta(k_1^2 + k_2^2 - k_3^2 - k_4^2)$. It is well-known that in the presence of impurities momentum conservation is violated. The transitions $\boldsymbol{k}, , k_2 \rightarrow k_3, k_4$ which involve the largest momentum transfer $(\approx 2k_F)$ are those which satisfy $\boldsymbol{k}, -k_2 = \mp(k_3 - k_4)$ and correspond to backscattering of both electrons $\boldsymbol{k}$, and k_2 to $k_4 = -k_1$ and

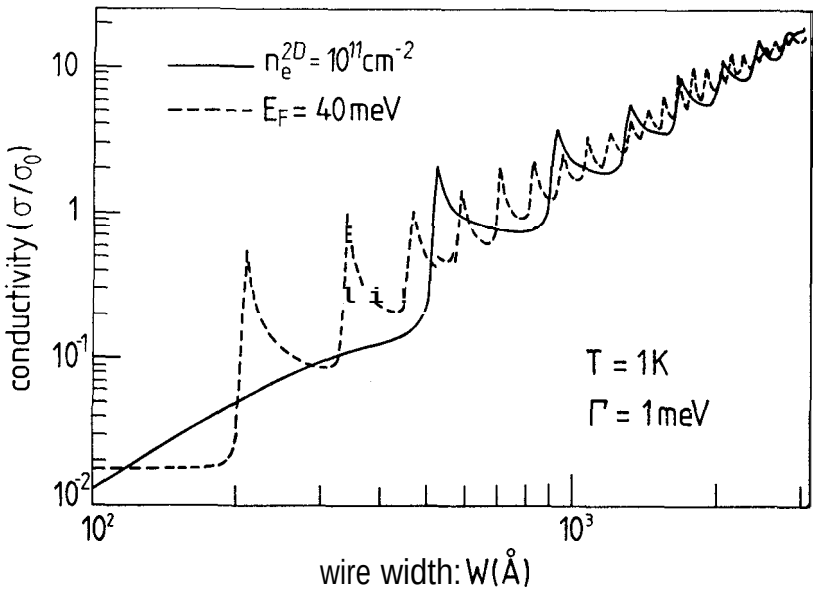

Fig.3 - The collisional contribution to the conductivity as a function of the width of the wire at fixed temperature and fixed level width. Two cases are considered: 1) the solid curve represents the situation for a conatant 2D electron density ($n_s^{2D} = n_e^{1D}/W = 10^{11} cm^{-2}$), and 2) the dashed curve is for the case in which the chemical potential is kept constant $E_F - 40\text{meV}$.

$k_3 = -k_2$(+sign) or $k_3 = -k_1$ and $k_4 = -k_2$ (−sign). Considering only those transitions which are expected to dominate the resistance, we obtain from eq.(3), near zero temperature

$$\sigma_c' \approx \sigma_2 \sum_n S(\epsilon_{F,n}, \Gamma_n) \int dk_3 f_{n,k_3}(1 - f_{n,k_3}) , \qquad (9)$$

where $\sigma_2 = (e^2/\hbar)(N_I U_0^2 F' l_e^2)(\sqrt{2}/4\pi k_\varsigma \Gamma)\sqrt{2m^*/\mathrm{h}^2}$, $F' = .26$. We see that eq.(9) has the same structure as eq.(7) and therefore shows the same oscillatory behavior as eq.(7). The amplitude, however, of the oscillations as estimated from the peak values of σ_c', i.e. when $E_F \to E_n + E_z^0$, is about 10 to 15 times smaller than the

corresponding amplitude of a_1 for T < 5K. Thus those collisions which involve backscattering of both electrons are very effective in reducing the conductivity. An order of magnitude estimate for the oscillation amplitude of the conductivity is obtained by adding the T $\rightarrow$ 0 expressions for σ_p and σ_c. Assuming $l_e \sim .5\mu m$, $m^* = .07m_0$, $k_s \approx 2 - 3/\AA$, and c $\approx .005/\AA$ we obtain $a_1 \approx 4 - 5 \times 10^{-6}$ and $\sigma_0 \approx 8 \times 10^{-6}$ in units of $(e^2/h)L[m]$. The precise values for σ_1 and σ_0 depend on the parameters N_I, k_s and c; both, however, decrease with N_I. This is apparent for σ_1, of eq.(6); for σ_0 it follows from the fact that increasing N_I leads to a decrease in 1, which makes the factor $N_I l_e^2$, in eq.(7), decrease for I, $\sim N_I^{-s}$, $s > .5$. With L $\sim 1\mu m$, these estimates lead to conductances of the observed order of magnitude[13].

In conclusion, we have present a calculation of the electrical conduction in quantum wires which: 1) is not limited to the size-quantum limit (n = O); ii) applies to δ function potentials as well as to the model potential $U_0 \exp(-k_s|x|)/\sqrt{|x|}$; iii) takes partially the electron-electron interaction into account, and iv) is valid both for square well and parabolic well confinement. Surface roughness scattering, boundary scattering, and a similar study in the presence of a magnetic field are left for future work. A study of magnetophonon resonances in quantum wires has already been completed[14].

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Resumo

Utiliza-se uma equação de Boltzmann *quântico* para calcular, a muito baixas temperaturas no regime de espalhamento por umpurezas, as contribuições difusiva e colisional à corrente elétrica dc ao longo de um fio quântico, de largura muito menor do que o livre caminho médio. Admite-se que os elétrons sejam independentes ou interajam (por colisóes binárias) na presença de impurezas. O confinamento lateral é modelado por um poço quadrado ou parabólico, e aquele na vertical por um poço triangular. Devido ao confinamento o movimento eletrônico torna-se quase-unidimensional e mudança na energia de Fermi ou na largura do fio levam a oscilações na densidade de estados, na taxa de espalhamento e na condutividade. O alargamento de níveis é levado em consideração auto-consistentemente.