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1990 J. Phys.: Condens. Matter 2 6743

(http://iopscience.iop.org/0953-8984/2/32/005)

J. Phys.: Condens. Matter **2** (1990) 6743–6754. Printed in the UK

Conductance of quantum wires with self-consistent level broadening

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Received 6 November 1989

Abstract. The non-equilibrium Green function technique is applied to derive a quantum kinetic equation for transport in quantum wires. Calculations are done for short-range impurity scattering neglecting localisation effects. In linear response the expression obtained for conductance is equivalent to the Kubo–Greenwood formula. Scattering-induced level broadening is included by self-consistent solution for the retarded Green function. For typical scattering strengths, level broadening suppresses oscillations of conductance in agreement with experimental observations. Width fluctuations of only 2% remarkably reduce quantum size effects, in arrays of parallel wires. A non-zero temperature ($T < 10$ K) is not limiting for observation of confinement effects in typical samples.

1. Introduction

Recently, extremely small conducting structures became technologically available. In such structures, one observes deviations from macroscopic transport properties due to the non-negligible influence of the wave character of electrons (Imry 1986). Semiconducting samples are of particular interest because of the possibility of changing the Fermi energy via the gate voltage and because of their importance for application. Quasi-one-dimensional (Q1D) samples are prepared mainly by imposing a lateral structure onto silicon MOSFETs (Warren *et al* 1986, Kastner *et al* 1987) or onto heterostructures from III–V compounds (Smith *et al* 1987, Alsmeier *et al* 1988, Brinkop *et al* 1988).

Plots of low-temperature conductance measurements show more or less pronounced structures with varying gate voltage. The relative fluctuations may be large for transport via hopping or resonant tunnelling in the region of strong localisation, $l_0 \ll L$, where l_0 and L denote the localisation length and the sample length, respectively (Fowler *et al* 1988). The fluctuations are smaller and of universal magnitude of e^2/h in the region of weak localisation where electron states are extended over the sample and transport is diffusive (Lee *et al* 1987). For this case the elastic scattering length l satisfies the condition $l \ll L \ll l_0$. The diffusive regime is only apparent if a sufficiently large number N of Q1D subbands is occupied by electrons since $l_0 \simeq Nl$. If l exceeds L, transport becomes ballistical and quantised steps are observed in the conductance versus gate voltage (van Wees *et al* 1988, Wharam *et al* 1988). These steps have been attributed to contact resistance (Imry 1986, Landauer 1987).

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In this paper we are concerned with the influence of quantum size effects (QSEs) in the diffusive region of transport. Universal fluctuations have been neglected, a situation which is met in arrays of parallel wires where fluctuations due to the sample-specific arrangement of impurities average out. This is equivalent to the case where the phase coherence length L_Φ is much smaller than the sample length L. The condition $L_\Phi \ll L$ (incoherent sample) is also sufficient to neglect the weak localisation correction to the average Boltzmann conductance which arises from the Born approximation in the one-electron self-energy. If impurities are the dominant sources of scattering the phase coherence length is also large compared with the elastic scattering length. Therefore the condition $l \ll L_\Phi \ll L, l_0$ has to be realised to observe QSEs as the main contribution to structures in conductance.

In the weak-scattering limit the QSEs should result in a vanishing conductance if the Fermi energy coincides with the botton of a subband. This is expected when the scattering rate is proportional to the Q1D density of final states. The consequences are large oscillations of conductance versus Fermi energy. The small magnitude of QSEs found in experiments (Warren *et al* 1986) indicates that the Boltzmann theory is inadequate for decribing these observations. Scattering-induced level broadening has to be included into a consistent transport theory for Q1D systems. This has been done in conductivity calculations starting from the Kubo–Greenwood formula (Das Sarma and Xie 1987, Kearney and Butcher 1987). However, the effects of renormalisation of the spectrum have been excluded from the beginning in these calculations and a diagonal approximation has been used in the expansion of the Green function with respect to subband wavefunctions.

In the following, a quantum kinetic equation for Q1D systems is derived using the non-equilibrium Green function technique as introduced by Kadanoff and Baym and by Keldysh. In sections 2–5 the theoretical formalism is applied to Q1D systems. Section 6 contains numerical results for dependence of the conductance on Fermi energy for different scattering strengths, fluctuations of channel widths and temperatures.

2. Model

Consider a quantum wire formed from a degenerate semiconductor of length L_x and rectangular cross section $A = L_y L_z$. The one-electron Hamiltonian of the wire without scattering is approximated by a simple one-band effective-mass model:

$$H_0(\bar{r}) = -(\hbar^2/2m^*)\nabla_x^2 + V_e(x) + H_c(r_\perp) \tag{1}$$

with the potential $V_e(x)$ of the electric field applied in the x direction (cf figure 1). We assume $V_e(x)$ to be decoupled from the confining potential $V_c(r_\perp)$ contained in the transverse part of the Hamiltonian:

$$H_c(r_\perp) = -(\hbar^2/2m^*)\nabla_{r_\perp}^2 + V_c(r_\perp). \tag{2}$$

Confinement results in quantisation of electron states in the two transverse directions according to

$$H_c(r_\perp)\varphi_\alpha(r_\perp) = E_\alpha \varphi_\alpha(r_\perp) \tag{3}$$

with discrete quantum numbers $\alpha = (n, m)$, subband energies E_α and real subband wavefunctions $\varphi_\alpha(r_\perp)$. The thermodynamic limit is performed in the x direction and, consequently, electrons are plane waves along the wire.

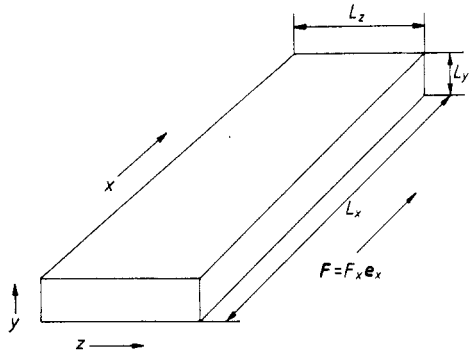

Figure 1. Schematic representation of the quantum wire and notations used in the text.

For sufficiently low temperatures, impurities are the dominant source of scattering. They are described by a random scattering potential $U(\boldsymbol{r})$ for which we use the model of Gaussian white noise:

$$\langle U(\boldsymbol{r})\rangle = 0 \qquad \langle U(\boldsymbol{r})U(\boldsymbol{r}')\rangle = g\delta(\boldsymbol{r}-\boldsymbol{r}'). \tag{4}$$

The average over all impurity configurations is denoted by $\langle \ldots \rangle$ and g is the coupling constant. For short-range scatterers of strength V_0, $g = nV_0^2$ where n is the volume density of scatterers.

3. Quantum kinetic equations

Transport equations including quantum effects may be derived by the non-equilibrium Green function technique. In this approach the usual perturbation theory is formulated in a complex time plane in non-equilibrium. Real-time quantities are obtained by analytical continuation which is performed very conveniently by applying the rules of Langreth and Wilkins (1972) and Langreth (1976). For the correlation function $G^<$ and the retarded function G_R, one obtains

$$[G_0^{-1} - \tilde{\Sigma}, G^<]_\pm - [\Sigma^<, \tilde{G}]_\pm = -(\mathrm{i}/2)[\Gamma, G^<]_\mp + (\mathrm{i}/2)[\Sigma^<, A]_\mp \tag{5}$$

and

$$[G_0^{-1}, G_R]_\pm = \mathbb{1} \pm \mathbb{1} + [\Sigma_R, G_R]_\pm. \tag{6}$$

Here, $[A, B]_\pm$ denote the anticommutator and commutator, respectively. In the spirit of a transport equation

$$G_0^{-1}(rt, r't') = \delta(\boldsymbol{r}-\boldsymbol{r}')\delta(t-t')[\mathrm{i}\,\partial/\partial t - \hbar^{-1}H_0(\boldsymbol{r})] \tag{7}$$

characterises the driving term in equations (5), and the right-hand side of equations (5) generalises the collision integral. The additional terms on the left-hand side of equations (5) describe renormalisation effects beyond the Boltzmann theory. The Dyson equation

for the retarded functions is generalised by equations (6). Furthermore we have used the definitions

$$A(rt, r't') = \mathrm{i}(G_\mathrm{R} - G_\mathrm{A})(rt, r't') \tag{8}$$

for the spectral function and

$$\tilde{G}(rt, r't') = \tfrac{1}{2}(G_\mathrm{R} + G_\mathrm{A})(rt, r't'). \tag{9}$$

Note that only two of equations (5) and (6) are independent.

Since we are interested in the average effect of impurity scattering only, equations (5) and (6) are written for averaged quantities without using a special notation. As a consequence of averaging, translational invariance in x direction is restored.

Scattering is described by replacing the impurity potential $U(\boldsymbol{r})$ by a complex non-local energy-dependent self-energy Σ. In the self-consistent Born approximation it may be written as

$$\Sigma(rt, r't') = \hbar^{-2}\langle U(\boldsymbol{r})U(\boldsymbol{r}')\rangle G(rt, r't') \tag{10}$$

which is valid for $\Sigma^<$, Σ_R and Σ_A. The self-energy parts Σ_R and Σ_A can be related to the spectral function Γ and the quantity $\tilde{\Sigma}$ in the same way as was done in equations (8) and (9).

In order to calculate the conductance G_QW of the quantum wire it is necessary to determine the current density

$$j(\boldsymbol{r}, t) = -(\hbar/m^*)(\nabla_{\boldsymbol{r}} - \nabla_{\boldsymbol{r}'})G^<(rt, r't)|_{\boldsymbol{r}'=\boldsymbol{r}} \tag{11}$$

which is connected with the conductance by

$$I_x = \int_A \mathrm{d}^2\boldsymbol{r}_\perp\, j_x(\boldsymbol{r}_\perp) = V_x G_\mathrm{QW} \tag{12}$$

in a stationary system homogeneous in the x direction. For a constant electric field F_x the potential difference is given by $V_x = F_x L_x$. Finally we introduce the particle density in the wire per length unit:

$$n(x, t) = -2\mathrm{i}\int_A \mathrm{d}^2\boldsymbol{r}_\perp\, G^<(rt, rt). \tag{13}$$

4. Equilibrium properties

In a linear response, carrier transport is determined by the equilibrium properties of the spectrum which will be discussed now.

In a homogeneous quantum wire the equilibrium quantities depend only on the relative variables $t - t'$ and $x - x'$ but separately on $\boldsymbol{r}_\perp$ and $\boldsymbol{r}'_\perp$ owing to inhomogeneity

in the transverse direction. After Fourier transformation of relative variables the retarded and advanced Green functions in the absence of scattering are

$$G^{(0)}_{R/A}(k_x, \omega; r_\perp, r'_\perp) = \sum_\alpha \varphi_\alpha(r_\perp)\varphi_\alpha(r'_\perp)(\omega - \varepsilon_{\alpha k_x} \pm \mathrm{i}0)^{-1} \tag{14}$$

with $\hbar\varepsilon_{\alpha k_x} = E_{\alpha k_x} = E_\alpha + \hbar^2 k_x^2/2m^*$. The corresponding spectral function

$$A_0(k_x, \omega; r_\perp, r'_\perp) = 2\pi \sum_\alpha \varphi_\alpha(r_\perp)\varphi_\alpha(r'_\perp)\delta(\omega - \varepsilon_{\alpha k_x}) \tag{15}$$

contains the sharp quasi-particle dispersion relation via the δ-function and its diagonal part in coordinate space determines the local density of states (LDOS)

$$\rho_0(\omega; r_\perp) = 2\sum_{\alpha k_x} \varphi_\alpha^2(r_\perp)\delta(\hbar\omega - E_{\alpha k_x}) = \frac{(2m^*)^{1/2}}{\pi\hbar} \sum_\alpha \varphi_\alpha^2(r_\perp)$$
$$\times (\hbar\omega - E_\alpha)^{-1/2}\theta(\hbar\omega - E_\alpha). \tag{16}$$

The latter shows the inverse square root behaviour with singularities at the bottoms of subbands characteristic of Q1D systems without scattering.

If scattering is present in the system, the retarded and advanced equilibrium Green functions obey the Dyson equation

$$(G_0^{eq})^{-1} G^{eq}_{R/A} = \mathbb{1} + \Sigma^{eq}_{R/A} G^{eq}_{R/A}. \tag{17}$$

Within our scattering model the self-energy is local in the transverse direction and independent of k_x in the self-consistent Born approximation:

$$\Sigma^{eq}_{R/A}(\omega; r_\perp, r'_\perp) = \delta(r_\perp - r'_\perp)\hat{\Sigma}^{eq}_{R/A}(\omega; r_\perp) \tag{18}$$

where

$$\hat{\Sigma}^{eq}_{R/A}(\omega; r_\perp) = \frac{g}{\hbar^2}\sum_{k_x} G^{eq}_{R/A}(k_x, \omega; r_\perp, r_\perp). \tag{19}$$

If no current flows from transverse to the wire, the Green functions are symmetric in the coordinates $r_\perp$ and $r'_\perp$ and the equilibrium spectral function is given by

$$A_{eq}(k_x, \omega; r_\perp, r'_\perp) = -2\,\mathrm{Im}\, G^{eq}_R(k_x, \omega; r_\perp, r'_\perp). \tag{20}$$

Furthermore one has

$$\tilde{G}_{eq}(k_x, \omega; r_\perp, r'_\perp) = \mathrm{Re}\, G^{eq}_R(k_x, \omega; r_\perp, r'_\perp). \tag{21}$$

Similar relations hold for the self-energy and

$$\hat{\Gamma}_{eq}(\omega; r_\perp) = -2\,\mathrm{Im}\,\hat{\Sigma}^{eq}_R(\omega; r_\perp) \tag{22}$$

is the scattering rate which determines the level broadening and depends upon the transverse position $r_\perp$. The LDOS in the presence of scattering given by

$$\rho(\omega; r_\perp) = \frac{1}{\pi\hbar}\sum_{k_x} A_{eq}(k_x, \omega; r_\perp, r_\perp) \tag{23}$$

is directly proportional to the scattering rate:

$$\hat{\Gamma}_{eq}(\omega; r_\perp) = (\pi g/\hbar)\rho(\omega; r_\perp). \tag{24}$$

The equilibrium correlation functions are

$$G^<_{eq}(k_x, \omega; r_\perp, r'_\perp) = \mathrm{i}\, A_{eq}(k_x, \omega; r_\perp, r'_\perp) f_0(\omega) \tag{25}$$

and

$$\hat{\Sigma}^<_{eq}(\omega; r_\perp) = \mathrm{i}\,\hat{\Gamma}_{eq}(\omega; r_\perp) f_0(\omega) \tag{26}$$

with the Fermi distribution function $f_0(\omega)$.

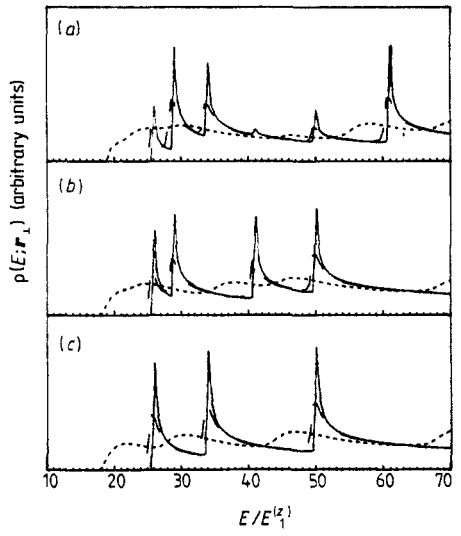

Figure 2. LDOS in a quantum wire at different positions $r_\perp$ ((*a*) (0.5 L_y, 0.23 L_z); (*b*) (0.5 L_y, 0.33 L_z); (*c*) (0.5 L_y, 0.5 L_z)) for three different scattering strengths $\beta = 0.01$ (——), $\beta = 0.1$ (— —) and $\beta = 1$ (– – –).

The Dyson equation (17), together with the functional dependence of the self-energy on the Green function as specified by equations (18) and (19), represents a set of equations which has to be solved self-consistently. In contrast with the bulk situation (Mahan 1987), the inhomogeneity in the transverse direction does not permit an exact formal solution for $G_{R/A}$ by Fourier transformation. A possible representation is an expansion with respect to the subband wavefunctions $\varphi_\alpha(r_\perp)$ which reflect the symmetry of the confining potential $V_c(r_\perp)$. Usually, the self-energy $\Sigma_{\alpha\alpha'}$ is approximated by its diagonal part (cf Kearney and Butcher 1987). The symmetry imposed by the confining potential is changed owing to interference between scattering and confinement, i.e. non-diagonal elements of $\Sigma_{\alpha\alpha'}$ are not necessarily negligible. We retain the diagonal approximation but include the change in symmetry by a parametric dependence of the self-energy on the transverse position. For $G^{eq}_{R/A}(r_\perp, r_\perp)$ our *ansatz* reads

$$G^{eq}_{R/A}(k_x, \omega; r_\perp, r_\perp) = \sum_\alpha \varphi^2_\alpha(r_\perp)\,[\omega - \varepsilon_{\alpha k_x} - \hat{\Sigma}^{eq}_{R/A}(\omega; r_\perp)]^{-1}. \qquad (27)$$

Note that this expression is consistent with equation (19). It is especially suited to the extremely short-range scattering mechanism considered here.

Using relation (27) the integral over k_x in equation (19) may be carried out analytically. The resulting implicit equation for $\Sigma_{R/A}$ is solved iteratively for each $r_\perp$ and ω. A regularisation procedure has to be employed in order to avoid unphysical contributions from large momenta to the real part of the self-energy (Serene and Rainer 1983). An additional valence band with the same effective mass has been introduced in order to cancel these contributions. This procedure does not affect level broadening.

Results for the LDOS are shown in figure 2 for several scattering strengths as specified by the dimensionless quantity $\beta = \hbar\Gamma^{2D}_B/2E^{(z)}_1$. The Boltzmann scattering rate $\Gamma^{2D}_B = mg/\hbar^3 L_y$ refers to a Q2D system of thickness L_y in the x–z plane in the electric quantum limit. The quantity $E^{(z)}_1$ is the energy of the first subband for hard-wall boundaries in the z direction and serves as energy unit in the following. For a typical width of the Q1D channel ($L_z \simeq 500$ Å), $E^{(z)}_1 \simeq 2$ meV and $\beta \simeq 1$ corresponds to a mobility μ^{2D}_B of

5×10^3 cm^2 V^{-1} s^{-1} in the reference system (low-mobility samples) whereas $\beta \simeq 0.01$ means that $\mu_B^{2D} \simeq 5 \times 10^5$ cm^2 V^{-1} s^{-1} (high-mobility samples). Throughout our calculation we have chosen wire dimensions of 100 Å × 500 Å. The energy range up to $70E_1^{(z)}$ covers the first subband in the y direction and six subbands in the z direction and encloses carrier concentrations up to 10^{12} cm^{-2} in the 2D reference structure. In the energy range between $30E_1^{(z)}$ and $70E_1^{(z)}$, $k_F^{2D} l_B^{2D} = 2E_F^{2D}/\hbar\Gamma_B^{2D} \simeq 2$–$20$ for $\beta = 1$ and $k_F^{2D} l_B^{2D} \simeq 2 \times 10^2$–$2 \times 10^3$ for $\beta = 0.01$ at $T = 0$ where $l_B^{2D} = v_F^{2D}/\Gamma_B^{2D}$ is the Boltzmann mean free path in the 2D system, E_F^{2D} is the Fermi energy measured from the first 2D subband, $E_1^y = \pi^2\hbar^2/2m^*L_y^2$, and k_F^{2D} and v_F^{2D} are the Fermi wavevector and velocity, respectively. This enables us to neglect strong-localisation effects in the above energy range for $\beta \leqslant 1$.

Figure 2 shows that the sharp peaks characteristic for the DOS of ideal Q1D wires are still present for high-mobility samples. In contrast, for structures with a low mobility typical of Si MOSFETs the peaks smear out and the DOS becomes similar to the 2D case. Renormalisation of the spectrum due to scattering manifests itself mainly in a rigid downshift in energy. The LDOS reflects directly the symmetry of the subband wavefunctions and contains position-dependent contributions of different subbands.

Using the relation

$$\rho(\omega; r_\perp)/\rho_{2D} = \hat{\Gamma}_{eq}(\omega; r_\perp)/\Gamma_B^{2D} \tag{28}$$

where $\rho_{2D} = m^*/\pi\hbar^2 L_y$ is the DOS of the 2D reference system; the local scattering rate may be obtained from figure 2. This permits comparison with experimental data, at least if scattering is short ranged.

5. Conductance

Generally, equations (5) and (6) possess a complicated structure because of the integration over internal space and time variables in each matrix product. Furthermore, the Dyson equation (6) becomes field dependent. The electric field introduces an inhomogeneity along the direction even in a homogeneous system. Therefore, it is convenient to eliminate the explicit dependence on the centre-of-mass coordinate $(x + x')/2$. This is always possible for a constant field via the transformation (Mahan 1987)

$$\Omega = \omega + (eF_x/\hbar)[(x + x')/2] \tag{29}$$

which considers the energy gain of a charge carrier caused by the field by tilting the spectrum.

The Fourier-transformed product of two quantities can be represented as

$$\mathcal{F}_{k_x\Omega}\{AB\} = \int_A \mathrm{d}^2 r''_\perp \, A(k_x, \Omega; r_\perp, r''_\perp)$$

$$\times \exp\left[\frac{\mathrm{i}}{2}\frac{eF_x}{\hbar}\left(\frac{\overleftarrow{\partial}}{\partial\Omega}\frac{\overrightarrow{\partial}}{\partial k_x} - \frac{\overleftarrow{\partial}}{\partial k_x}\frac{\overrightarrow{\partial}}{\partial\Omega}\right)\right] B(k_x, \Omega; r''_\perp, r'_\perp) \tag{30}$$

in a stationary case and for a system homogeneous in the x direction. The arrows indicate that derivatives act to the left or to the right, respectively. Linear response requires consideration of the first two terms in an expansion of the exponent in equation (30).

This means that in a linear response a rigorous solution is obtained by the gradient expansion often used in quantum transport theory for slowly varying disturbances (Kadanoff and Baym 1962). Note that no gradient expansion has been performed in the transverse direction.

Current flow in the x direction and the extremely short-range scattering mechanism further simplify the expressions since only quantities diagonal in the transverse position $\boldsymbol{r}_\perp$ are necessary. In this case, equation (6) with anticommutators leads to the relation

$$(eF_x/\hbar)\{[1-(\partial/\partial\Omega)\hat{\Sigma}_R(\Omega;\boldsymbol{r}_\perp)](\partial/\partial k_x)+v_x(\partial/\partial\Omega)\}G_R(k_x,\Omega;\boldsymbol{r}_\perp,\boldsymbol{r}_\perp)=0 \tag{31}$$

for the diagonal retarded function. The equilibrium Dyson equation follows from equation (6) for commutators up to corrections quadratic in electric field. We conclude similar to the bulk case (Mahan 1987) that the retarded Green function diagonal in the transverse position $\boldsymbol{r}_\perp$ has no contributions linear in the electric field:

$$G_R^{F_x}(k_x,\Omega;\boldsymbol{r}_\perp,\boldsymbol{r}_\perp)=G_R^{eq}(k_x,\Omega;\boldsymbol{r}_\perp,\boldsymbol{r}_\perp)+O(F_x^2) \tag{32}$$

in the stationary case and for a system homogeneous in the x direction. Relation (32) does not hold generally for the non-diagonal part in the transverse direction which would give rise to additional terms in the conductance for non-local scattering.

Next, equation (5) is treated in an analogous way, yielding an expression for the correlation function $\delta G^<(k_x,\Omega,\boldsymbol{r}_\perp,\boldsymbol{r}_\perp)$ linear in the electric field. The procedure is similar to that performed in the bulk case (Mahan 1987). The resulting equation contains contributions proportional to the Fermi function itself in addition to the usual terms proportional to its derivative. Taking the imaginary part of equation (31) it can be shown that the contributions proportional to the Fermi function cancel each other exactly. Note that this is a consequence of taking into account the renormalisation terms in equation (5). For isotropic scattering, vertex corrections to the conductance disappear, i.e. the last anticommutator on the right-hand side of equation (5) possesses no term linear in the electric field. In the Boltzmann theory this is equivalent to coincidence of the inverse scattering rate and transport relaxation time. As a result, $\delta G^<$ can be expressed as

$$\delta G^<(k_x,\Omega;\boldsymbol{r}_\perp,\boldsymbol{r}_\perp)=i(eF_x/\hbar)[-\partial f_0(\Omega)/\partial\Omega]\hat{\Gamma}_{eq}^{-1}(\Omega;\boldsymbol{r}_\perp)$$
$$\otimes\{v_xA_{eq}(k_x,\Omega;\boldsymbol{r}_\perp,\boldsymbol{r}_\perp)-\hat{\Gamma}_{eq}(\Omega;\boldsymbol{r}_\perp)(\partial/\partial k_x)[\mathrm{Re}\,G_R^{eq}(k_x,\Omega;\boldsymbol{r}_\perp,\boldsymbol{r}_\perp)]\}. \tag{33}$$

Using the relation between conductance and correlation function in the form

$$G_{QW}=\frac{2e}{iF_xL_x}\int_A d^2\boldsymbol{r}_\perp\sum_{k_x,\Omega}v_x\delta G^<(k_x,\Omega;\boldsymbol{r}_\perp,\boldsymbol{r}_\perp) \tag{34}$$

we find for the conductance of a quantum wire

$$G_{QW}=\frac{2e^2}{\hbar L_x}\sum_{k_x\Omega}\left(-\frac{\partial f_0(\Omega)}{\partial\Omega}\right)\int_A d^2\boldsymbol{r}_\perp\,\hat{\Gamma}_{eq}^{-1}(\Omega;\boldsymbol{r}_\perp)$$
$$\otimes[v_x^2A_{eq}(k_x,\Omega;\boldsymbol{r}_\perp,\boldsymbol{r}_\perp)+\frac{\hbar}{m^*}\hat{\Gamma}_{eq}(\Omega;\boldsymbol{r}_\perp)\,\mathrm{Re}\,G_R(k_x,\Omega;\boldsymbol{r}_\perp,\boldsymbol{r}_\perp)]. \tag{35}$$

This is the central analytical result of the paper. It is justified if the system can be

considered homogeneous in wire direction and if the self-energy is a local quantity. Equation (35) coincides with the result from the Kubo–Greenwood formula

$$G_{QW} = \frac{e^2}{\hbar L_x} \sum_{k_x \Omega} \left(-\frac{\partial f_0(\Omega)}{\partial \Omega} \right) \int_A d^2 r_\perp \, d^2 r'_\perp \, v_x A_{eq}(k_x, \Omega; r_\perp, r'_\perp) v_x A_{eq}(k_x, \Omega; r'_\perp, r_\perp). \tag{36}$$

The expression obtained by Kearney and Butcher (1987) is recovered if a subband expansion for the spectral function is carried out in equation (36) with subsequent diagonal approximation in subband indices. Equation (35), however, is better suited to apply the *ansatz* (27) since it contains quantities diagonal in the transverse position $r_\perp$ only.

We complete this section with a discussion of the Boltzmann limit for weak scattering. In this case we retain the most divergent terms in equation (35). The self-consistent inverse scattering rate is replaced by its first iteration $\hat{\Gamma}_B^{-1}$ proportional to the DOS calculated from equation (16). The spectral function approaches its value without scattering (equation (15)). No divergence arises from the term proportional to the real part of the Green function and this term can be neglected. The quantity $\hat{\Gamma}_B^{-1}$ is the position-dependent relaxation time in the Boltzmann theory as analysed by Ziep *et al* (1986) and by Pratsch and Suhrke 1988, 1989) for the Q2D case. It can be easily verified that

$$G_{QW}^B = \frac{2e^2}{L_x} \sum_{\alpha k_x} v_x^2 \left(-\frac{\partial f_0(E_{\alpha k_x})}{\partial E_{\alpha k_x}} \right) \tau_\alpha(E_{\alpha k_x}) \tag{37}$$

with the subband relaxation time

$$\tau_\alpha(E_{\alpha k_x}) = \int_A d^2 r_\perp \, \varphi_\alpha^2(r_\perp) \hat{\Gamma}_B^{-1}(E_{\alpha k_x}; r_\perp). \tag{38}$$

It should be noted that equation (38) differs from the usual results of the Boltzmann theory for low-dimensional systems based on Fermi's golden rule for the transition probability (Ando *et al* 1982). In this case the inverse subband relaxation time

$$\tau_\alpha^{-1}(E_{\alpha k_x}) = \int_A d^2 r_\perp \, \varphi_\alpha^2(r_\perp) \hat{\Gamma}_B(E_{\alpha k_x}; r_\perp) \tag{39}$$

arises from integration over the cross section already in the transport equation. This may lead to remarkable differences in the dependence of conductance on temperature and carrier concentration (Ziep *et al* 1986, Pratsch and Suhrke 1988, 1989).

6. Results and discussion

The position-dependent conductance including the self-consistent level broadening is shown in figure 3 for the same sequence of parameters as in figure 2 and for zero temperature. The conductance is measured in units of $(e^2/\beta h)(L_y/L_x)$. The length-dependent factor has been introduced in order to obtain an intensive quantity. The conductance unit $e^2/\beta h$ is related to the two-dimensional reference system again and is simply its Boltzmann conductance multiplied by $E_1^{(z)}/E_F^{2D}$. The position dependence of the conductance is a reminiscent of the inhomogeneous distribution of charge carriers over the cross section as discussed in section 4.

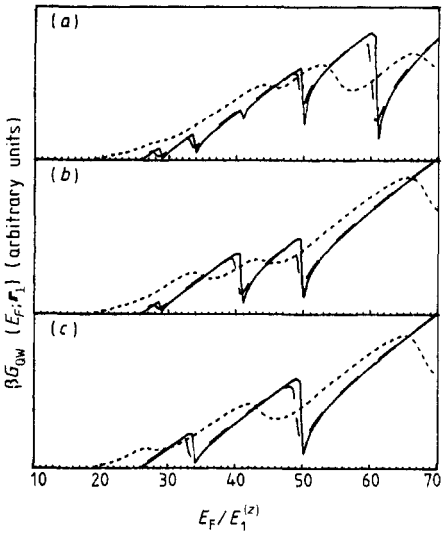

Figure 3. Position-dependent contributions to conductance for the same parameters as in figure 2 ($T = 0$ K).

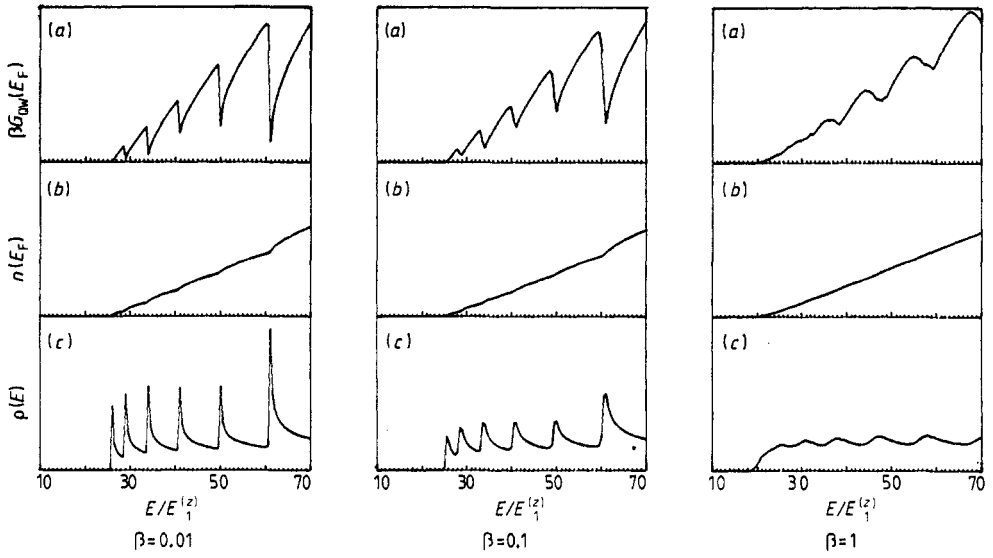

Figure 4. (*a*) Conductance and (*b*) number of carriers for a quantum wire and (*c*) the total DOS for three different scattering strengths.

Figure 4 shows the dependences of the total conductance and the number of carriers in the wire per length unit (which both depend on the Fermi energy) and the averaged DOS on $E/E_1^{(z)}$ for the same parameters as above. For weak scattering ($\beta \simeq 0.01$–0.1) the conductance exhibits strong oscillations with the Fermi energy known from the Boltzmann theory. This Q1D behaviour is also seen in the carrier concentration and DOS. The oscillations disappear almost completely for strong scattering and the physics become nearly like those in a 2D system. This is especially pronounced in the low-energy

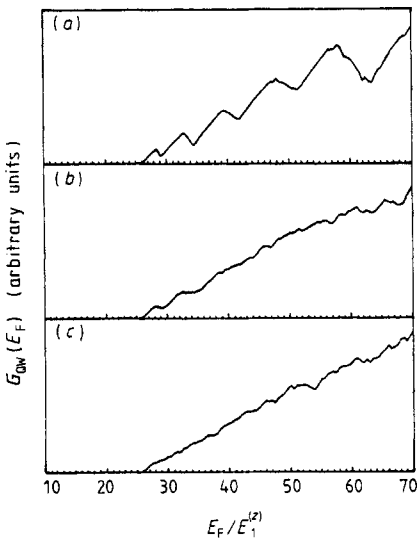

Figure 5. Influence of width fluctuations on the conductance for an array of quantum wires as shown by the conductance versus Fermi energy plots for RMS deviations fron $L_z = 500$ Å of (*a*) 2%, (*b*) 5% and (*c*) 10% ($\beta = 0.1$; $T = 0$ K).

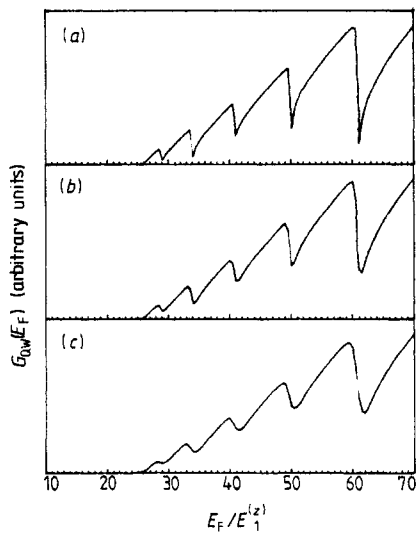

Figure 6. Influence of finite temperature on the conductance of a quantum wire for (*a*) $T = 0$ K, (*b*) $T = 4.2$ K and (*c*) $T = 10$ K ($\beta = 0.1$).

region where the level broadening is of the same order of magnitude as subband separation. As a result, scattering-induced level broadening limits the observation of QSEs in low-mobility ($\mu_{2D} \leqslant 10^4$ cm^2 V^{-1} s^{-1} samples (Warren *et al* 1986, Kastner *et al* 1987).

QSEs are expected to dominate in arrays of parallel channels obtained by the grating–gate technique (Warren *et al* 1986) because sample-specific universal fluctuations are averaged out. On the other hand, conductance oscillations due to the confinement should become less pronounced, too, because of the differences in properties from wire to wire. The influence of width fluctuations is analysed in figure 5 under otherwise ideal conditions (high-mobility sample at zero temperature). The channel widths L_z in the grating direction are assumed to be normally distributed around the average value of 500 Å. Fluctuations of only 2% lead to a significant reduction in size effects. They vanish almost completely for fluctuations of about 10%. This value coincides with estimations from experiments on silicon MOSFETs (Warren *et al* 1986). Characteristic values for GaAs/$Ga_{1-x}Al_xAs$ heterostructures are 5% (Smith *et al* 1987).

Finally, figure 6 shows that, under proper conditions, confinement-induced oscillations of conductance are clearly resolved for temperatures up to 10 K, i.e. if thermal broadening is smaller than level spacing.

Generally, our results confirm that QSEs are observable if the characteristic broadening in energy does not exceed the level spacing.

We conclude with some remarks on the applicability of our calculations. They are suited to the structures used in recent experiments (Warren *et al* 1986, Smith *et al* 1987, Alsmeier *et al* 1988, Brinkop *et al* 1988). In these structures obtained by the grating technique, always a sufficient number of Q1D subbands is occupied and the conditions mentioned in the introduction are fulfilled. Structures imposed on silicon inversion

layers are not such good candidates for observation of subband structure because of their low mobility. Samples based on III–V compounds, on the other hand, possess a higher mobility and a lower effective mass, leading to a larger subband spacing which makes QSEs more accessible.

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