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Coherent-potential approach for the zero-temperature DC conductance of weakly disordered narrow systems

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Abstract. The configurationally averaged zero-temperature DC conductance of weakly disordered systems of finite width is calculated using the coherent-potential approximation. There is no smooth transition from the quantised quasi-ballistic regime at low disorder to the structureless conductance for larger disorder. Instead the conductance oscillates as a function of the Fermi energy in the intermediate region. The perturbation theory agrees well with the numerical results obtained previously.

1. Introduction

Recent transport experiments on small metallic systems at low temperatures have provided a number of new and interesting phenomena that can be assigned to the coherence of the quantum mechanical states of the electrons. One of these phenomena consists of the 'universal conductance fluctuations' in the diffusive regime of impure metals (for a review see [1]). These fluctuations are of the order of e^2/h and are independent of the geometry and of the microscopic nature of the sample. On the contrary, in the ballistic regime where the elastic mean free path l of the electrons is at least comparable with or even much greater than the geometrical dimensions of the system, the low-temperature DC conductance $\Gamma(0)$ shows well defined plateaux as a function of the width of the system and the magnetic field, the plateau values being integer multiples of e^2/h [2]. The quantised behaviour of the conductance was explained as a consequence of the quantisation of the transverse components of the wavevectors of the electrons in a narrow constriction between two wide conducting regions [3]. Explicit theoretical calculations [4–6] for narrow quasi-one-dimensional (quasi-1D) systems, (width M) have confirmed the exact quantisation that is independent of the length L of the system and of the specific form of the confining potential. The conditions for quantisation in narrow constrictions of various shapes have been investigated by several researchers [7–10].

Having in mind the special features of Γ in the two asymptotic regions $l \gg L$ and $l \ll L$, one can ask what its behaviour in the intermediate case is. Our recent numerical calculations [6] showed that the configurationally averaged conductance of weakly

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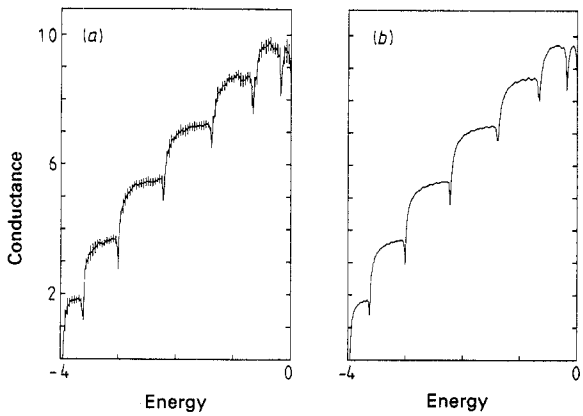

Figure 1. Conductance in units of e^2/h as a function of the Fermi energy in units of V, the off-diagonal part of the Hamiltonian. (*a*) Results of numerical calculations [6] for $M = 15$, $L = 100$, $W = 0.4V$. The average conductance (several hundreds of samples) is shown as a full line. The RMS deviations are indicated by vertical lines. (*b*) Result of the CPA calculation for the same parameters.

disordered systems of finite width is still quantised, the plateau values being approximately equidistant, and the height of the steps exceeds the RMS deviation of Γ. However, the steps are smoothed by the disorder, and their height is smaller than e^2/h. In addition, a remarkable decrease in the conductance just below any step was observed (figure 1(*a*)). We have interpreted this effect as a result of a disorder-induced hybridisation of the sub-bands. One should also be able to describe these 'anti-resonances' using perturbation theory, in order to gain better insight into the underlying physics.

This is what we want to achieve in this paper. We shall use a coherent-potential approximation (CPA) technique [11] for the description of tunnelling through a disordered barrier (see also [12]), and apply it to our model for the transport in systems of finite widths. We shall be able to explain in more detail the origin of the anti-resonances, and to describe the non-trivial transition between the quantised and the smooth behaviour of the conductance when the disorder is increased.

2. Coherent-potential approximation for the conductance

We consider a quasi-1D system which consists of a disordered part of the length L and of two perfectly conducting infinite leads connected to its ends. We want to calculate the averaged conductance, assuming that, if an infinitesimal voltage is applied to the system, the electric field is non-zero only in its finite part involving disorder. We call this part the sample.

The DC conductance is [5, 6, 13, 14]

$$\Gamma = -(h/8\pi^2 L^2)\,\mathrm{Tr}[J^{(\mathrm{sample})}\,\Delta G(E_\mathrm{F})\,J^{(\mathrm{sample})}\,\Delta G(E_\mathrm{F})] \tag{1}$$

where $J^{(\mathrm{sample})}$ denotes the operator of the current density spatially averaged over the part of the system with a non-zero electric field. We take the field as constant within the sample because the DC response depends only on the total voltage and not on the distribution of the field [6, 14, 15]. $G^{\pm}(E) = (E \pm \mathrm{i}0 - H)^{-1}$ are the one-particle Green functions, and $\Delta G = G^{+} - G^{-}$.

To be specific, we take a square lattice M lattice spacings wide and use a tight-binding representation of the Hamiltonian

$$H = \sum_{\mathrm{NN}} |lm\rangle\langle l'm'| + \sum_{l,m} |lm\rangle \varepsilon_{lm} \langle lm| \tag{2}$$

and of the current operator

$$J^{(\mathrm{sample})} = \frac{e}{\mathrm{i}h} \sum_{l=1}^{L} J^{(l)} \tag{3}$$

$$J^{(l)} = \sum_{m=1}^{M} (|lm\rangle\langle l-1m| - |l-1m\rangle\langle lm|). \tag{4}$$

Here $\{|lm\rangle\}$ is a complete set of orthonormal states associated with the lattice sites. The stochastic potential is non-zero within the sample ($1 \leqslant l \leqslant L$) only. It is represented by the random site energies ε_{lm}.

We transform equation (1) into a form more convenient for the averaging. First we use the current conservation expressed by an operator identity

$$\Delta G\,(J^{(l)} - J^{(l')})\,\Delta G = 0 \tag{5}$$

to avoid the summation involved in equation (4):

$$\Gamma = (e^2/2h)\,\mathrm{Tr}(J^{(1)}\,\Delta G\,J^{(L+1)}\,\Delta G). \tag{6}$$

Then, using the sub-band representation $\{|l\mu\rangle\}$ and the multiplicative form of the matrix elements of the Green function in the one-dimensional sub-bands, we obtain

$$\Gamma = (e^2/h)\,\mathrm{Tr}[C^{(1)}G^{+}(E_{\mathrm{F}})C^{(L)}G^{-}(E_{\mathrm{F}})] \tag{7}$$

where

$$C^{(l)} = \sum_{\mu=1}^{M} |l\mu\rangle v_{\mu} \langle l\mu| \tag{8}$$

and v_μ is the Fermi velocity in the μth sub-band. Equation (7) is simply an invariant transcription of the multi-channel conductance formula [13, 14].

The evaluation of the configurationally averaged conductance equation (7) within the CPA [11] consists of two steps. Firstly, the averaged one-particle Green function $\langle G(z)\rangle$ is constructed by replacing the random part V of the Hamiltonian equation (2) by a self-energy operator $\Sigma(z)$ which is diagonal in the site representation. In the weak-disorder limit when the CPA reduces to the self-consistent Born approximation (SCBA), the matrix elements of the self-energy operator are

$$\sigma_{lm}(z) = w^2 \langle lm|G(z)|lm\rangle \tag{9}$$

with $w^2 = \langle \varepsilon_{lm}^2 \rangle$. Because of the inhomogeneity in the l direction due to the leads, $\sigma_{lm}(z)$ depends on the layer index l. It does not depend on m if we use, for simplicity, the periodic boundary condition in the transverse direction, because the averaging then

restores the equivalence of all sites within a layer. Then $\langle G(z)\rangle \equiv G(z)$ is diagonal in the 1D-sub-band representation. We define

$$G_{l,l'}(\mu, z) = \sum_{m=1}^{M} \langle l0|G(z)|l'm\rangle \exp\left(\frac{2\pi i\mu m}{M}\right) \tag{10}$$

so that

$$\sigma_l(z) = w^2 \frac{1}{M} \sum_{\mu=1}^{M} G_{l,l}(\mu, z). \tag{11}$$

The operators $C^{(1)}$ and $C^{(L)}$ in equation (7) are non-random quantities so that the averaging of the conductance means the averaging of the direct product of two Green functions. Following [11], we denote

$$K = \langle G^+(E_F)C^{(L)}G^-(E_F)\rangle. \tag{12}$$

The averaging of the product equation (12) cannot be reduced to replacing V by $\Sigma(z)$. Doing this, i.e. averaging the two Green functions separately, we obtain only the coherent part of K, i.e.

$$K^C = G^+(E_F)C^{(L)}G^-(E_F) \tag{13}$$

and of the conductance, i.e.

$$\Gamma^C = \frac{e^2}{h} \sum_{\mu=1}^{M} v_\mu^2 |G^+_{1,L}(\mu, E_F)|^2. \tag{14}$$

The weak-disorder limit of the full set of the CPA equations for K (equations (49) and (50) in [11]) consistent with the approximation in equation (9) reads [11, 12]

$$K = G^+(E_F)\left(C^{(L)} + \sum_{l=1}^{L}\sum_{m=1}^{M} |lm\rangle\, w^2\langle lm|K|lm\rangle\langle lm|\right) G^-(E_F). \tag{15}$$

Because of the periodic boundary conditions in the m direction the diagonal elements of K do not depend on m: $\langle lm|K|lm\rangle = K_l$. Rewriting equation (15) in the sub-band representation, we obtain a matrix equation for K_l:

$$K_l - \sum_{l'=1}^{L} w^2 A_{l,l'} K_{l'} = K_l^C \tag{16}$$

where the matrix **A** consists of the elements [12]

$$A_{l,l'} = \frac{1}{M} \sum_{\mu=1}^{M} |G^+_{l,l'}(\mu, E_F)|^2. \tag{17}$$

Substituting the solution of equation (16) into equation (15), we obtain the final CPA expression for the averaged conductance:

$$\Gamma = (e^2/h)\,\mathrm{Tr}(C^{(l)}K) = \Gamma^C + \Gamma^V. \tag{18}$$

The incoherent part Γ^V of the conductance ('vertex correction') is [12]

$$\Gamma^V = \frac{Me^2}{h} \sum_{l,l'=1}^{L} R_l \left(\frac{w^2}{1 - w^2 A}\right)_{l,l'} L_{l'} \tag{19}$$

with

$$R_l = \frac{1}{M}\sum_{\mu=1}^{M} v_\mu |G^+_{L,l}(\mu, E_F)|^2 \tag{20}$$

$$L_l = \frac{1}{M}\sum_{\mu=1}^{M} v_\mu |G^+_{l,l}(\mu, E_F)|^2. \tag{21}$$

Both R_l and L_l contain the contributions of the 1D sub-bands in a sum. Therefore Γ^V, as well as Γ^C, can be uniquely decomposed into contributions corresponding to the electron transmission from one sub-band on the left, μ, to another one on the right, μ'. These individual contributions are just the averaged transmission probabilities appearing in the multi-channel conductance formula [16].

3. Results

Equations (10)–(21) can be evaluated straightforwardly. We assume that the random atomic levels ε_{lm} are distributed uniformly within the interval $(-W/2, W/2)$ so that a direct comparison with the results of the numerical calculations [6] is possible. The second moment of the distribution function $P(\varepsilon)$ is then $w^2 = W^2/12$. The higher moments of $P(\varepsilon)$ do not appear in the SCBA equations (11) and (12), derived for the case of weak disorder, but they define the validity range of the approximation. In the particular case of the box distribution the SCBA gives almost the same results as the full CPA even for moderately strong disorder, as we shall see shortly.

To illustrate the behaviour of the averaged conductance of the narrow disordered channel, we take first $M = 15$, $L = 100$, $W = 0.4V$. Figure 1 shows the dependence of Γ on the Fermi energy.

There is a remarkably good agreement between the 'exact' result of the numerical calculation (figure 1(*a*)) and the SCBA (figure 1(*b*)). In particular, the 'dips' separating the 'plateaux' are clearly resolved. This indicates that the anti-resonances reflect a basic mean-field property of the narrow weakly disordered channels. The question is whether or not it is a density-of-states (DOS) effect.

The DOS has a series of 1D van Hove singularities at the edges of the sub-bands for vanishing disorder, $W = 0$. They are smoothed to a certain degree but are still present for $W \neq 0$ if the disorder is not too large, i.e. $W \ll 4V$, the width of the unperturbed sub-bands. There is no indication of an anti-resonance at the energy of the onset of a new sub-band in the DOS as can be seen in figure 2. Thus the anti-resonances in the conductance cannot be a DOS effect in the usual sense and must result from the energy dependence of the mobility.

The lifetime of the carriers is inversely proportional to the imaginary part of the self-energy. This quantity has, according to (9), the same structure as the DOS. It means that the mobility of the electrons, and correspondingly also the conductance, is strongly reduced whenever the Fermi energy approaches the edge of a new sub-band. The underlying physics is simple; the scattering cross section for the electron is proportional to the number of available states into which it can be scattered by the disorder, so that the energy dependence of the conductance involves a 'negative' DOS. This can be seen more explicitly if we look at the sub-band contributions to the conductance:

$$\Gamma_\mu = \sum_\nu \Gamma_{\mu\nu}. \tag{22}$$

Figure 2(*b*) shows the contribution Γ_1 of the lowest sub-band as a function of the Fermi

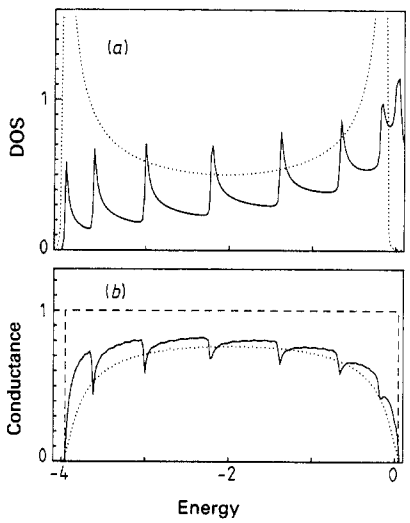

Figure 2. (*a*) Average density of states in arbitrary units and (*b*) conductance in units of e^2/h of the lowest sub-band as a function of the Fermi energy in units of V, the off-diagonal part of the Hamiltonian. The parameters are $M = 15$, $W = 0.4V$. The corresponding 1D results are shown as dotted lines.

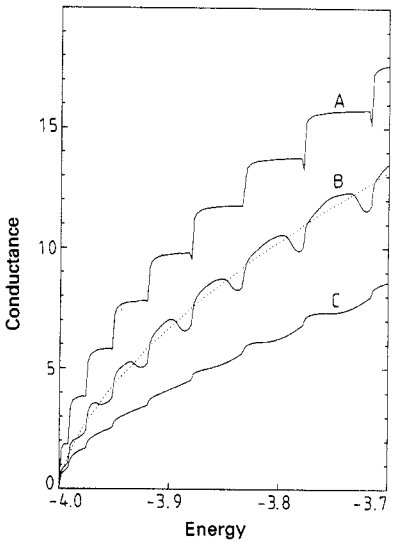

Figure 3. Average conductance as obtained from the CPA approach in units if e^2/h as a function of the Fermi energy in units of V for $M = 99$, $W = 0.1V$ (curve A), $W = 0.5V$ (curve B), and $W = 1V$ (curve C). For comparison the corresponding result for $M = 2000$ is shown as a dotted line for curve B.

energy and, for comparison, also the smooth conductance corresponding to $M = 1$. A more detailed discussion of the role of the non-diagonal processes (cf equation (19)) will be given elsewhere [15].

In order to be closer to the experimental situation we have also studied the conductance of wider channels with only a few lowest channels occupied. For realistic values of M ($M \simeq 10^3$) the sub-band offsets become so small that only the effects of rather weak randomness can be visualised without destroying the conductance quantisation. Figure 3 summarises the results for $M = 99$ for $W = 0.1V$ (curve A), $W = 0.5V$ (curve B) and $W = 1V$ (curve C). In the first case, Γ is still well quantised although the steps are rounded. The anti-resonances are extremely narrow, such that they cannot be resolved energetically. In the intermediate case the disorder is strong enough to destroy the plateaux. The anti-resonances survive; their width becomes comparable with the distance between successive sub-band edges. As a result the conductance shows strong oscillations as a function of the Fermi energy. The dips mark the positions of the sub-band edges. For comparison, we have also shown the result for $M = 2000$ (rescaled) where the transverse quantisation becomes unimportant, and Γ increases monotonically with increasing Fermi energy, as in the 2D diffusive regime. In the limit of strong disorder (figure 3, curve C) almost all the structure in Γ has vanished.

4. Conclusion

It should be possible to observe the disorder-induced conductance oscillations in samples and at temperatures where the quantised behaviour is seen. By careful ion bom-

bardment, one can damage the samples weakly. It is clear that the disorder-induced oscillatory behaviour of Γ should also be observed when the width of the system is changed, or when a magnetic field is applied. We expect that oscillatory behaviour of the average of Γ will be observed for a given sample since the expected statistical fluctuations will be much smaller than e^2/h (universal conductance fluctuations [1], of the order of unity on the scale of figure 3).

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