THEORY OF THE QUANTUM BALLISTIC TRANSPORT IN CONSTRICTIONS AND QUANTUM RESONANCE DEVICES

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INTRODUCTION

Recent experimental developments on quantized conductance in 2D point contacts (1) have prompted a flurry of theoretical activity (2) in the field of quantum ballistic transport. Although the theoretical approaches differ in various respects, they all have in common that they are based on, or can be traced back to, the Landauer formula

$$G=e^2/h \sum_{ij} T_{ij} \qquad (1)$$

which applies to an idealized two-terminal geometry. A detailed discussion about the consequences of applying this formula to non-ideal geometries, e.g. having a finite width of the wide parts of the sample, was given by Landauer (3). Also in the present paper I will stick to idealized geometries, where the microstructure is flanked by infinite 2D halfplanes. The electrical contacts to these planes are assumed to lie far from the constriction(s) compared to the inelastic mean free path.

The formalism underlying the numerical results that I will discuss below is given in Ref. 4. In the present paper I will only briefly point out the basic physics. The linear conductance through a constricted region in an otherwise unperturbed 2DEG can be calculated from the eigenfunctions in the following way: Due to the presence of a constriction the eigenfunctions having their principle weight in the left half plane (left-side lobes) contribute an infinitesimal leakage current through the constriction. Similarly the right-side lobes contribute a particle current pointing to the left. In the absence of an external voltage these currents cancel. Due to a small external voltage between left and right the left-side lobes will acquire a surplus

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occupation given by the density of states multiplied by the change in potential. The resulting current is now given by this extra density multiplied with the flux of each eigenfunction (i.e. the rate at which a unit area passes from left to right) integrated over all left-side lobes. For the left-side and right-side lobes the angle of incidence is still a good quantum number, which is due to the infinite extent of the continuum solutions compared to the finite scattering cross section of the constriction. Therefore the summation over eigenstates in terms of an angular integral can be expressed as follows:

$$G = e^2 \int_{-\pi/2}^{\pi/2} \Phi(E_F,\alpha)\ \frac{\partial^2 n}{\partial E \partial \alpha}\ d\alpha \qquad (2)$$

A set of tight binding wave functions is used to represent the electronic states, which is convenient for computational reasons and has the possibility of working in the limit of free electron bands ($\lambda_F >> a$, a is the lattice parameter) and nonparabolic bands ($\lambda_F \approx a$). The Hilbert space is a 2D square lattice with nearest neighbor hopping parameter t, which corresponds to $\hbar^2 / (2\, m^* a^2)$ where m^* is the effective mass near the center of the Brillouin zone. For such a tight binding lattice the flux can be expressed in the value of the eigenfunctions at two adjacent rows of lattice points, which can be chosen at x=0 and x=a respectively (The x and y directions are chosen perpendicular and parrallel to the barrier respectively) :

$$\Phi(\psi) = \frac{4\pi t a^2}{h}\ \mathrm{Im}\left(\sum_n \langle\psi|0,n\rangle \langle 1,n|\psi\rangle\right) \qquad (3)$$

In Ref. 4 it was shown, that in a geometry with a set of apertures in an infinetely high barrier at x = 0 the conductance is exactly given by:

$$G = \frac{2e^2}{h}\ \mathrm{Tr}\{(\mathrm{Im}\Gamma^*)\ (\mathrm{Im}\Gamma^{-1}) \qquad (4)$$

where

$$\Gamma_{n,n'} \equiv \pi^{-1} \int_0^{\pi} \cos([n-n']\phi)\ \sqrt{(E/2t - 2 + \cos(\phi))^2 - 1}\ d\phi$$

In the more general case, where a microstructure (a tube with or without delta function impurities, a box, a horn etc.) is added to the aperture(s), the expression is slightly more complicated. A detailed description is given in Ref. 4. Part of the results discussed below were calculated with the latter expression.

II. CONDUCTANCE QUANTIZATION IN POINTCONTACTS

In Fig. 1 the result is given for a few configurations where the conductance as a function of constriction width is calculated. The following observations can be made from this figure:

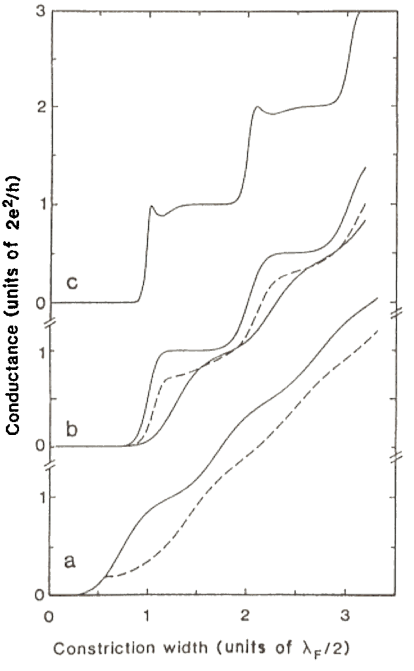

Fig.1. Conductance versus constriction width. (a)L=0. Solid/dashed curve: constriction without/with impurity. (b)L=0.48λ_F. Upper solid curve: channel without impurity. Lower solid curve: impurity inside the constriction (x=0.32λ_F, y=0.32λ_F). Dashed curve: impurity outside the constriction (x=0.57λ_F, y=0.32λ_F). (c)L=0.99λ_F.

In the first place there are oscillations with inflection points at precise integer multiples of $2e^2/h$ even for a constriction of zero length. On increasing the length of the constriction the plateaus start to flatten, until at a critical length L_c the plateaus become horizontal. On further increasing the length oscillations below the plateaus set in due to interference between waves reflected from the back and front end of the narrow region. The critical length where the n'th plateau becomes horizontal obeys the following scaling behaviour :

$$L_c = 0.45 \sqrt{W\lambda_F} = 0.32\, \lambda_F \sqrt{n} \qquad (5)$$

The square root dependance of L_c on W implies that in order to have quantization the narrow region can be much shorter than wide. Note that this is somewhat counter intuitive: In order to have 1D subbands one tends to assume that a channel must be much longer than wide. This turns out to be an unnecessary condition. More important is, that the channel length is of the order of (or smaller than) the decay length $1/\kappa$ of the electrons tunnelling below the lowest unoccupied 1D subband in the narrow region, i.e. $L_c^{-2} \sim \kappa^2 \sim 2m\hbar^2 (E_{n+1} - E_n)$. In a square well confinement potential the latter energy difference is propertional to the channel index: $\kappa^2 \sim n\, W^{-2}$. Using the fact, that the channel index n is approximately given by $2W / \lambda_F$ we can now qualitatively understand, that L_c is proportional to the square root of the width. Also shown in Fig.1 is the effect of impurities, which clearly is to destroy quantization.

III. QUANTUM RESONANCE DEVICES

I now turn to the problem of a small box connected to 2D half planes on both sides through point contacts. Technically such a device can be realized by means of a set of gates that defines the shape, and a second gate covering the box and its surroundings. The latter gate can be used to define the position of the Fermi level. In Fig. 2 the result is given for a round box. The peaks coincide with the energy positions of the localized levels inside the box and are caused by resonant tunneling. In the situation depicted in Fig. 2 the apertures on both sides act as mode selectors which allow only for partial transmission of the lowest subband in the narrow region. This effectively makes the problem 1D, even though the continuum states to which the localized states in the box couple are in the 2D half planes. The only relevant quantum number is now parity with respect to the y mirror plane. The states can be characterized by 'atomic' quantum numbers: 1s, $1p_x$, $1d_{x^2-y^2}$, 2s etc. . For a box of 200 nm diameter and an effective mass of $0.07m_e$ these levels are at 3.6, 9.3, 16.7 and 18.5 K respectively. The $1p_x$ and $1d_{x^2-y^2}$ levels are degenerate with the $1p_y$ and $1d_{xy}$ levels respectively, but the latter do not couple to the modes selected by the point contacts, as these levels have odd symmetry around the x-axis, whereas the selected modes are even. With regards to mirror symmetry around the y axis we observe, that 1s, $1d_{x^2-y^2}$ and 2s are even, whereas $1p_x$ is odd.

As parity is conserved by the coupling of the localized states to the continuum (The slight asymmetry in the geometry of Fig. 2 has neglegible physical influence) one can write $|k_p\rangle = (|-k_R\rangle \pm |k_L\rangle)/\sqrt{2}$, where p indicates the parity quantum number and the +/- sign refers to even and odd parity. In(out) coming waves have posive (negative) values for k. Due to unitarity the outcoming waves acquire a parity- and energy-dependent phase shift $\eta_p(E)$. A wave entering from the left is given by a linear combination of even and odd-parity waves, so that the scattered wave is: $|k_{scatt}\rangle = 2^{-1/2} (e^{2i\eta_e} |k_e\rangle + e^{2i\eta_o} |k_o\rangle)$. The transmission is now:

$$T = |\langle -k_R | k_{scatt}\rangle|^2 = \sin^2(\eta_e - \eta_o) \qquad (6)$$

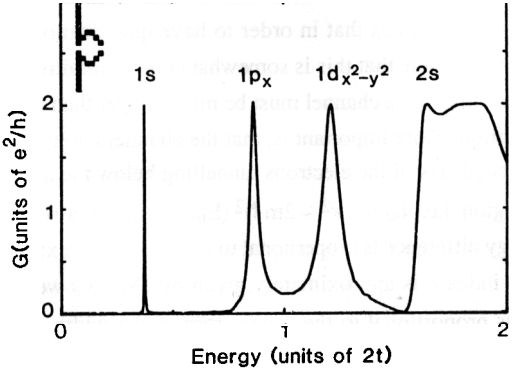

Fig.2. Conductance versus Fermi energy for the geometry indicated in the top left corner. In the calculation the barrier extends from y = -∞ to ∞. Indicated above each resonance are the orbital quantum numbers of the corresponding virtual bound states.

In the more general case of an asymmetrical box other linear combinations of L and R waves have to be taken, which results in a reduced transmitted amplitude compared to Eq. (6). The energy dependance of the phase shifts follows directly from the Friedel Sum Rule (5):

$$d\eta_p / dE = \pi \Delta\rho_p \tag{7}$$

where $\Delta\rho_p$ is the impurity induced change in the density of states. Generally speaking this implies, that the phase shift increases with π each time the Fermi level crosses a quasi localized level, giving rise to a resonance peak with a maximum transmission of exactly one. If an even and an odd level are energetically close to each other, complete or partial cancellation can occur. On the other hand, if there is a succession of two or more states of the same parity, there must be a point of exactly zero transmission between two subsequent peaks. Especially if the energy positions are close to each other this gives rise to a very strong energy dependency of the conductance. In its simplest form the change in density of states connected with each localized state has a Lorentzian line shape:

$$\Delta\rho_p = \pi \frac{d}{dE} \mathrm{Arg}(E - E_{ip} - i\,\Gamma_{ip}) \tag{8}$$

This immediately leads to the following form of the phase shifts:

$$\eta_p = \sum_i \mathrm{cotg}^{-1}(\Gamma_{ip} / (E - E_{ip})) \tag{9}$$

A plot of η_e, η_o, η_e-η_o and T is displayed in Fig. 3 , taking 3, 14, and 18 K for the energy position of the even peaks and 0.2, 1.5 and 2.0 K for the corresponding Γ. The odd peak was positioned at 7K with Γ=1.0 K. Clearly most of the physics of Fig.2 is contained in the simple scattering phase shift considerations explained above.

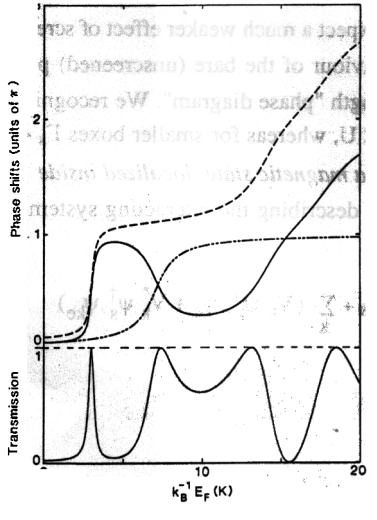

Fig. 3 . The phase shifts and the transmission versus Fermi energy of a QRD containing 3 even levels and 1 odd level. Dashed, chained and solid curves are η_e, η_o and η_e- η_o .

IV. ELECTRON CORRELATION IN QRD'S

So far I have neglected electron correlation effects. Although this is reasonable in the 2D wide parts of the geometry, as interactions are strongly screened there, this is no longer correct in a small box, or even in a 1D constriction. Especially in a small box the situation is reminiscent to atomic physics. Let us first take a look at the relevant energy scales. We take the energy difference between the two lowest levels (1s and 1p) as representative of the level spacings without electron-electron interactions:

$$\Delta E = E_p - E_s = \frac{\hbar^2}{2\ m^*}\ \frac{0.71}{\pi\ R^2} \tag{10}$$

the width of the s level scales as

$$\Gamma_s \approx E_s\ \frac{W}{R}\ \exp(-2\pi\ \frac{L}{W}\ \sqrt{1 - \frac{2W^2}{\pi R^2}}\ ) \tag{11}$$

i.e., keeping the shape and the relative sizes of the QRD fixed, the linewidths and the energies scale with R in the same way. The Coulomb integral of two electrons in a 2D circular box scales as:

$$U = f\ \frac{e^2}{\varepsilon R} \tag{12}$$

where ε is the dielectric constant and f is a dimensionless factor of the order one which depends on the details of the wavefunctions involved. If two electrons occupy states with different orbital quantum numbers, we also have to take into account the exchange integral J, favouring parallel spin alignment. The exchange integral follows the scaling behaviour of the unscreened Coulomb interaction U given in Eq. (12). Both an increase of the number of occupied levels and a reduction of ΔE leads to a reduced value of U due to screening. From the analogy with transition metal impurities I expect a much weaker effect of screening on the exchange interaction J (6). The scaling behaviour of the bare (unscreened) parameters is displayed in Fig. 4 in a temperature versus length "phase diagram". We recognize from this plot, that for boxes larger than 110 (nm) $\Delta E < U$, whereas for smaller boxes $\Gamma_s << U < \Delta E$. *The latter condition leads to the formation of a magnetic state localized inside the box on partial filling of the s level.* The Hamiltonian describing the interacting system is the well known Anderson impurity Hamiltonian:

$$H = \sum_k \varepsilon_k\ \psi_{ke}^{\dagger}\ \psi_{ke} + \sum_\sigma n_{\sigma s} + U\ n_{\downarrow s} n_{\uparrow s} + \sum_k\ (V_k\ \psi_{ke}^{\dagger}\ \psi_s + V_k^*\ \psi_s^{\dagger}\ \psi_{ke}) \tag{13}$$

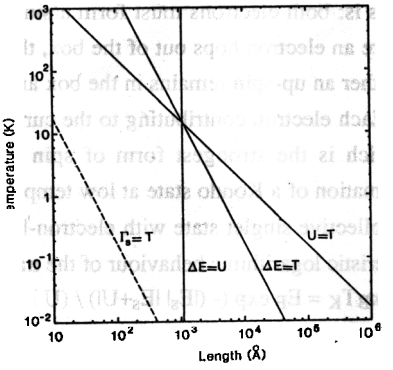

Fig. 4. Phase diagram of temperature versus diameter of a circular QRD (using typical GaAs parameters for the effective mass and the dielectric constant), indicating the various regions in parameter space.

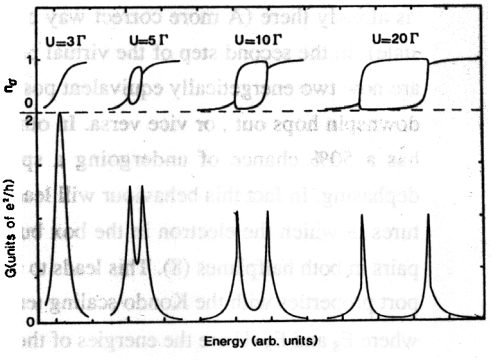

Fig. 5. Plot of the conductance (lower panel) and the occupation number for both spin directions in the localized state (upper panel) versus Fermi energy for various values of U/Γ.

The easiest approximation is to solve the Schrodinger equation using the self consistent Hartree-Fock approximation (7). As a result the s-virtual bound state will divide up in two spin split peaks as soon as the density of states at the Fermi level exceeds a certain critical value. This can only occur if $U > \pi\Gamma$. In other words, if the latter so called Anderson criterion is fulfilled, the Hartree-Fock approximation gives a sharp transition between the magnetic and the non magnetic regime as a function of s-level occupation. It is important to point out that this sharp transition is an artifact of the Hartree-Fock approximation. More advanced ground state calculations lead to a gradual crossover between the two regimes (8). I have performed the selfconsistent Hartree-Fock calculation as a function of Fermi energy, thus extracting a conductance per spin channel from the s-level occupation numbers (i.e. by employing the Friedel sum rule). The resulting conductances and occupation numbers are displayed in Fig. 5. The leftmost example is at the border of the above mentioned Anderson criterion and there is only a single peak with its maximum at $2e^2/h$. For larger U the Anderson criterion is satisfied and there are now two peaks, with their maxima between e^2/h and $2e^2/h$.

The rightmost example is representative of the box of about 200 nm diameter discussed in section 3. If in this example the Fermi level is inbetween the two peaks, the box contains approximately a single spin, and we have to face the fact, that our previous assumption of independent channels for the two different spin quantum numbers no longer holds. The reason is as follows: A current flowing through the box has to be envisaged as a sequence of virtual hops of electrons and/or holes into and out of the box. An applied voltage favours hopping in one direction. An electron hopping into the box must have its spin antiparallel to the spin that

is already there (A more correct way of stating this is: both electrons must form a singlet state). In the second step of the virtual process, where an electron hops out of the box, there are now two energetically equivalent possiblities: Either an up-spin remains in the box and a downspin hops out , or vice versa. In other words: Each electron contributing to the current has a 50% chance of undergoing a spin flip, which is the strongest form of spin flip dephasing. In fact this behaviour will lead to the formation of a Kondo state at low temperatures in which the electron in the box builds up a collective singlet state with electron-hole pairs in both halfplanes (8). This leads to the characteristic logarithmic behaviour of the transport properties with the Kondo scaling temperature: $k_B T_K = E_F \exp(-(|E_s|\,|E_s+U|) / (U\,\Gamma_s))$, where E_s and E_s+U are the energies of the occupied and the unoccupied spin levels relative to the Fermi energy. With the gated QRD structure one has the unique possibility of tuning these energies and hence of having an experimental handle on T_K. In the case where the Fermi level is precisely midway E_s and E_s+U, one can easily estimate that the Kondo temperature is far below experimentally accessible temperatures. On moving the Fermi level closer to one of the peaks T_K rises sharply and the anomalous temperature dependency should enter the observable temperature range. Therefore I believe, that Quantum Resonance Devices are a unique tool for studying collective behaviour induced by spin flip scattering.

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