Anomalies in the conduction edge of quantum wires

T. Rejec[1], A. Ramšak[1,2] and J.H. Jefferson[3]

[1] *J. Stefan Institute, SI-1000 Ljubljana, Slovenia*

[2] *Faculty of Mathematics and Physics, University of Ljubljana, SI-1000 Ljubljana, Slovenia*

[3] *DERA, St. Andrews Road, Great Malvern, Worcestershire WR14 3PS, England*

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We study the conductance threshold of clean nearly straight quantum wires in which an electron is bound. We show that such a system exhibits spin-dependent conductance structures on the rising edge to the first conductance plateau, one near $0.25(2e^2/h)$, related to a singlet resonance, and one near $0.75(2e^2/h)$, related to a triplet resonance. As a quantitative example we solve exactly the scattering problem for two-electrons in a wire with circular cross-section and a weak bulge. From the scattering matrix we determine conductance via the Landauer-Büttiker formalism. The conductance anomalies are robust and survive to temperatures of a few degrees. With increasing magnetic field the conductance exhibits a plateau at e^2/h, consistent with recent experiments.

I. INTRODUCTION

Following the pioneering work in Refs. [1,2] many groups have now observed conductance steps in various types of quantum wire. These first experiments were performed on gated two-dimensional electron gas (2DEG) structures, while similar behaviour of conductance are shown in "hard-confined" quantum wire structures, produced by cleaved edge over-growth [3], epitaxial growth on ridges [4], heteroepitaxial growth on "v"-groove surfaces [5] and most recently in GaAs/Al$_\delta$Ga$_{1-\delta}$As narrow "v"-groove [6] and low-disorder [7] quantum wires.

These experiments strongly support the idea of ballistic conductance in quantum wires and are in surprising agreement with the now standard Landauer-Büttiker formalism [8,9] neglecting electron interactions [10]. However, there are certain anomalies, some of which are believed to be related to electron-electron interactions and appear to be spin-dependent. In particular, already in early experiments a structure is seen in the rising edge of the conductance curve [1], starting at around $0.7G_0$ with $G_0 = 2e^2/h$ and merging with the first conductance plateau with increasing energy. Under increasing in-plane magnetic field, the structure moves down, eventually merging with a new conductance plateau at e^2/h in very high fields [11,12]. Theoretically this anomaly has not been adequately explained, despite several scenarios, including spin-polarised sub-bands [13], conductance suppression in a Luttinger liquid with repulsive interaction and disorder [14] or local spin-polarised density-functional theory [15]. Recently we have shown that these conductance anomalies near $0.7G_0$ and $0.25G_0$ are consistent with an electron being weakly bound in wires of circular and rectangular cross-section, giving rise to spin-dependent scattering resonances [16–18].

In this paper we develop further the single bound-electron picture and give new results for wires of circular cross-section, including magnetic field dependence.

II. THE MODEL

We consider quantum wires which are almost perfect but for which there is a very weak effective potential, which has at most two bound states. Such an effective potential can arise, for example, from a smooth potential due to remote gates. Alternatively it could arise from a slight buldge in the an otherwise perfect wire. We consider this latter situation for the cases of quantum wires with both circular cross-section [16], appropriate for 'hard-confined' v-groove wires; or rectangular cross-section [17], which approximate 'soft-confined' wires resulting from gated 2DEGs. These are shown schematically in Figure 1. The cross-sections of these wires are sufficiently small that the lowest transverse channel approximation is adequate for the energy and temperature range of interest. The smooth variation in cross-section also guarantees that inter-channel mixing is negligible. Restricting ourselves to this lowest transverse channel, the Schrödinger equation on a finite-difference grid in the z-direction may be written,

$$H = -t \sum_{i\sigma} \left(c_{i+1,\sigma}^\dagger c_{i\sigma} + c_{i\sigma}^\dagger c_{i+1\sigma} \right) + \sum_{i\sigma} \epsilon_{i\sigma} n_{i\sigma} + \sum_i U_{ii} n_{i\uparrow} n_{i\downarrow} + \frac{1}{2} \sum_{i\neq j} U_{ij} n_i n_j, \tag{1}$$
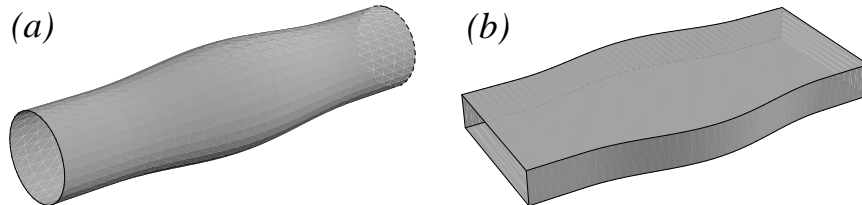
FIG. 1. The wire shape is symmetric around the z-axis. The potential is constant $V(x,y,z) = 0$ within the boundary, and $V_0 > 0$ elsewhere. (a) Circular cross-section, defined by, $r_0(z) = \frac{1}{2}a_0(1 + \xi \cos^2 \pi z/a_1)$ for $|z| \leq \frac{1}{2}a_1$ and $x_0(z) \equiv \frac{1}{2}a_0$ otherwise. (b) Rectangular cross-section is defined by $x_0(z) = \frac{1}{2}a_0(1 + \xi \cos^2 \pi z/a_1)$.

where $c_{i\sigma}^{\dagger}$ creates an electron with spin σ at the $z = z_i$ in the lowest transverse channel; $n_i = \sum_{\sigma} n_{i\sigma}$ with $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$; $t = \hbar^2/(2m^*\Delta^2)$, where $\Delta = z_{i+1} - z_i$; $\epsilon_i = \hbar^2/(m^*\Delta^2) + \epsilon(z_i+) + g^*\mu_B\sigma B$, where $\epsilon(z_i)$ is the energy of the lowest transverse channel at z_i and $g^*\mu_B\sigma B$ is the Zeeman energy for a magnetic field B in the z-direction, as in Refs. [16,17]. U_{ij} is an effective screened Coulomb interaction which was obtained by starting with a full 3D Coulomb interaction, integrating over the lowest transverse modes and then adding screening phenomenologically. The dielectric constant is taken as $\varepsilon = 12.5$, appropriate for GaAs. Note that this is a general form, the difference between the two cases shown in Figure 1 being reflected entirely in the energy parameters ϵ and U. We note that this Hamiltonian also has the form for a perfectly straight wire subject to a smooth potential variation, defined by the ϵ.

III. TWO-ELECTRON APPROXIMATION

Over a range of parameters in which the deviation from a perfect straight wire is small, one, and only one, electron resides in a bound state. This is because the weak effective potential provided by the bulge will always contain at least one bound state and since the binding energy is small, a second electron cannot be bound due to Coulomb repulsion. For larger bulges or deeper potential wells more electrons may be bound but these situations will not be considered here. Note that even if there is more than one bound state (we consider one or two) there can still only be one bound electron due to the Coulomb repulsion. The actual number of electrons in the wire may be changed by varying the Fermi energies in the leads and reservoirs to which the wire is connected. In experiments, this is achieved simply by changing the voltages on one or more gate electrodes. When there is more than one electron in the wire, a current will flow from source to drain contacts and at low temperatures the motion of these electrons is ballistic. The conduction electrons will scatter from the bound electron giving rise to resistance. If we neglect the mutual interaction between conduction electrons, then the transport problem reduces to a two-electron scattering problem described by equation (1). This is a reasonable approximation provided that the mean electron density is not too low, i.e. that the mean electron separation is of order the effective Bohr radius or less. We solve the two-electron scattering problem exactly subject to the boundary condition that the asymptotic states consist of one bound electron in the ground state and one free electron. The main features of these scattering solutions may be understood by the following simple physical picture. The effective potential due to the single bound electron and the effective potential well gives rise to a symmetric double barrier structure since an incident electron will initially feel the Coulomb repulsion due to the bound electron but will then pass through a weak local minimum, e.g., at the the point of maximum diameter in the wire of circular cross-section. This gives rise to a resonance, the peak of which corresponds to perfect transmission. A more refined analysis shows that this resonance is spin dependent, singlet and triplet resonances occuring at different energies, with the singlet always lowest. In fact this spin-dependent scattering is the quasi one-dimensional analogue of the three-dimensional case, discussed some 70 years ago by Oppenheimer and Mott [19].

From the scattering solutions we compute the conductance using again a Landauer-Büttiker formula which, incorporating the results of spin-dependent scattering, takes the following form,

$$G = -\frac{2e^2}{h} \int \frac{\partial f(\epsilon - E, T)}{\partial \epsilon} \left[\frac{1}{4}[\mathcal{T}_s(\epsilon - E_B) + \mathcal{T}_t(\epsilon - E_B)] + \frac{1}{2}\mathcal{T}_t(\epsilon + E_B)\right] d\epsilon \tag{2}$$

where the subscripts $\mathcal{T}_s$ and $\mathcal{T}_t$ refer to singlet and triplet transmission probabilities respectively, with $E_B = \frac{1}{2}g^*\mu_B B$ and E is the Fermi energy in the leads.

IV. RESULTS

We have performed detailed calculations for both the circular and rectangular wire cross sections shown in Figure 1. Apart from small quantitative differences, the results are very similar and hence, for brevity, we shall only show results for wires with circular cross-section.

In Fig. 2(a) we show plots at zero temperature and magnetic field of $\mathcal{T}_s(E)$ and $\mathcal{T}_t(E)$ for a typical wire with the geometry of Fig. 1(a). The thin dotted line represents the non-interacting result, independent of spin. We see clearly the sharp singlet resonance at low energy followed by the broader triplet at higher energy. In Fig. 2(b) the conductance G in units of $2e^2/h$ is shown, as calculated for various temperatures. The resonances have a strong temperature dependence and, in particular, the sharper singlet resonance is more readily washed out at finite temperatures. However, it should be noted that resonances survive to relatively high temperatures, because the width of the wire, which dictates the energy scale, is small ($a_0 = 10$ nm) [20]. Note that for weak coupling, the energy scale is set by the x-energy of the lowest channel, $\sim a_0^{-2}$ and hence the conductance vs. Ea_0^2 with Ua_0 fixed is roughly independent of a_0 (the scaling would be exact for $V_0 \to \infty$).
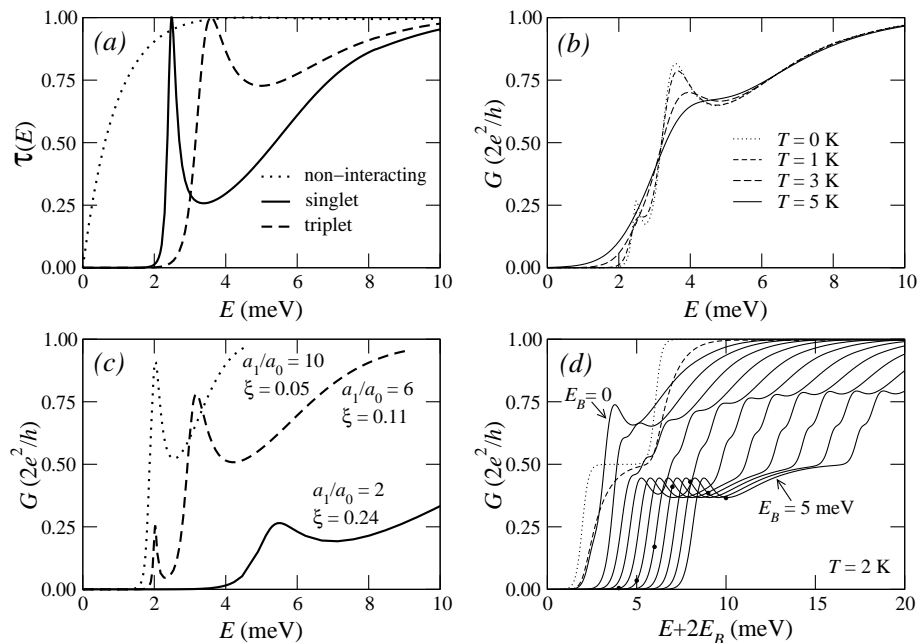

FIG. 2. Resonance and conductance curves. (a) Typical transmission probabilities for singlet and triplet resonances in zero magnetic field. Here [and in (b) and (d)] $a_0 = 10$ nm, $a_1 = 60$ nm, $\xi = 0.1$ and $V_0 = 0.4$ eV. (b) Total conductance in zero magnetic field showing temperature dependence of anomalies near 0.25 and 0.7. (c) Dependence of conductance on wire geometry. (d) Magnetic field dependence of conductance showing weak resonance and saturation to e^2/h in a high magnetic field.

In Fig. 2(c) we show the zero temperature and field conductance curves for three different bulge shapes, which become longer and flatter as we move from right to left. For the case with the shortest bulge region (right) we see only a singlet resonance. This is because the effective potential well has only one bound state and hence, even in the absence of Coulomb interaction, would not support a triplet. On the other hand, the other two cases have two one-electron bound states. In the absence of Coulomb interaction, these levels give rise to singlet and triplet bound states. When the Coulomb interaction is switched on, the states develop into two resonance peaks (dotted line). Here the position of both peaks nearly coincides, because the buldge is relatively long and the singlet-triplet splitting is small. For the remaining case (dashed line), both the lowest singlet and triplet develop into resonances when the Coulomb interaction is switched on, though the singlet is only just unbound with the resonance lying close to the conduction edge energy and is thus very sharp.

In Fig. 2(d) conductance for $T = 2$ K is presented for magnetic field increasing from zero in steps with $\Delta E_B = 0.5$ meV and for clarity the curves have been shifted by $2E_B$ to the right with increasing E_B. We present results for $a_0 = 10$ nm, but note that E_B also obeys the above mentioned scaling $E_B a_0^2$ with varying a_0. Magnetic fields which would give substantial effects in e.g. narrow "v"-groove wires [6], would have to be very large, since $E_B = 1$ meV

corresponds to large $g^*B \sim 35$ T. However, due to "$E_B a_0^2$" scaling, the corresponding value for a wider wire with $a_0 \sim 50$ nm would be only ~ 1.4 T. Also plotted in Fig. 2(d) for comparison are the corresponding results for the non-interacting electron case (dotted) and the perfectly straight wire (dashed), with $E_B = 2$ meV. In this figure we have indicated with a dot the points $E = E_B$. To the left of these points G simplifies, $G(E, B) = \frac{e^2}{h} \mathcal{T}_t(E + E_B)$, whereas at high energies spin-flip transmission probabilities $t_{\uparrow\downarrow\to\uparrow\downarrow}$ and $t_{\uparrow\downarrow\to\downarrow\uparrow}$, contained within the remaining terms of Eq. (2), are non-zero. These parts of the curves should be treated with caution though they are expected to be more reliable at lower fields.

V. SUMMARY

In summary, we have shown that quantum wires with weak longitudinal confinement, or open quantum dots, can give rise to spin-dependent, Coulomb blockade resonances when a single electron is bound in the confined region. The emergence of a specific structure at $G(E) \sim \frac{1}{4}G_0$ and $G \sim \frac{3}{4}G_0$ is a consequence of the singlet and triplet nature of the resonances and the probability ratio 1:3 for singlet and triplet scattering and as such is a universal effect. A comprehensive numerical investigation of open quantum dots using a wide range of parameters shows that singlet resonances are always at lower energies than the triplets, in accordance with the corresponding theorem for bound states [21]. With increasing in-plane magnetic field, the resonances shift their position and a plateau $G(E) \sim e^2/h$ emerges. The effect of a magnetic field is observable only in relatively wider quantum wires, due to the intrinsic energy scale $\propto a_0^{-2}$.

[1] B.J. van Wees *et al.*, Phys. Rev. Lett. **60**, 848 (1988).
[2] D.A. Wharam *et al.*, J. Phys. C **21**, L209 (1988).
[3] A. Yacoby *et al.*, Phys. Rev. Lett. **77**, 4612 (1996).
[4] P. Ramvall *et al.*, Appl. Phys. Lett. **71**, 918 (1997).
[5] M. Walther, E. Kapon, D.M. Hwang, E. Colas, and L. Nunes, Phys. Rev. B **45**, 6333 (1992); M. Grundmann *et al.*, Semicond. Sci. Tech. **9**, 1939 (1994); R. Rinaldi *et al.*, Phys. Rev. Lett. **73**, 2899 (1994).
[6] D. Kaufman *et al.*, Phys. Rev. B **59**, R10433 (1999).
[7] B.E. Kane *et al.*, Appl. Phys. Lett. **72**, 3506 (1998); D.J. Reilly, cond-mat/0001174.
[8] R. Landauer, IBM J. Res. Dev. **1**, 223 (1957); **32**, 306 (1988).
[9] M. Büttiker, Phys. Rev. Lett. **57**, 1761 (1986).
[10] H. van Houten, C.W.J. Beenakker, and B.J. van Wees, in *Semiconductors and Semmimetals*, edited by R.K. Willardson, A.C. Beer, and E.R. Weber, (Academic Press, 1992).
[11] K.J. Thomas *et al.*, Phys. Rev. Lett. **77**, 135 (1996); Phys. Rev. B **58**, 4846 (1998); **59**, 12252 (1999).
[12] K.J. Thomas *et al.*, Phil. Mag. B **77**, 1213 (1998).
[13] G. Fasol and H. Sakaki, Jpn. J. Appl. Phys. **33**, 879 (1994).
[14] D.L. Maslov, Phys. Rev. B **52**, R14368, 1995.
[15] Chuan-Kui Wang and K.-F. Berggren, Phys. Rev. B **57**, 4552 (1998).
[16] T. Rejec, A. Ramšak, and J.H. Jefferson, cond-mat/9910399.
[17] T. Rejec, A. Ramšak, and J.H. Jefferson, J. Phys.: Condens. Matter **12**, L233 (2000).
[18] V.V. Flambaum and M.Yu. Kuchiev, cond-mat/9910415.
[19] J.R. Oppenheimer, Phys. Rev. **32**, 361 (1928); N.F. Mott, Proc. Roy. Soc. A **126**, 259 (1930).
[20] A. Ramšak, T. Rejec, and J. H. Jefferson, Phys. Rev. B **58**, 4014 (1998).
[21] E. Lieb and D. Mattis, Phys. Rev. **125**, 164 (1962).