

Interacting electrons in a nearly straight quantum wire

T. Rejec¹, A. Ramšak^{1,2}, and J.H. Jefferson³

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*

(July 26, 2000)

We study the conductance threshold of a clean nearly straight quantum wire in which a single electron is bound. This exhibits spin-dependent conductance anomalies on the rising edge to the first conductance plateau, near $G = 0.25(2e^2/h)$ and $G = 0.7(2e^2/h)$, related to a singlet and triplet resonances respectively. We show that the problem may be mapped on to an Anderson-type of Hamiltonian and calculate the energy dependence of the energy parameters in the resulting model.

Conductance steps in various types of quantum wire have now been observed, following the pioneering work in Refs. [1]. These first experiments were performed on gated two-dimensional electron gas (2DEG) structures, though similar behaviour has now been observed in other quantum wire structures [2]. Whilst these experiments strongly support the idea of ballistic conductance in quantum wires, and are in surprising agreement with the now standard Landauer-Büttiker formalism [3], certain anomalies can arise which are spin-dependent and are believed to originate from electron-electron interactions. In particular, already in early experiments a structure is seen in the rising edge of the conductance curve [1], starting at around $0.7(2e^2/h)$ and merging with the first conductance plateau with increasing energy. Later experiments also clearly showed anomalies near $G = 0.25(2e^2/h)$ [2]. Recently we have shown that these conductance anomalies are consistent with an electron being weakly bound in wires of circular and rectangular cross-section, giving rise to spin-dependent scattering resonances [4].

In this paper we present further results on the above anomalies, related to singlet and triplet resonances for a propagating electron at the Fermi energy scattering from the weakly bound electron. This two-electron problem (solved exactly) is then mapped onto a many-electron Anderson-type model for which the most important matrix elements are retained.

We consider quantum wires which are almost perfect but for which there is a very weak effective potential, giving rise to a bound state. Such an effective potential can arise, for example, from a smooth potential due to remote gates or a slight buldge in an otherwise perfect wire. We consider this latter situation for the cases of quantum wires with circular cross-section, appropriate for, e.g., ‘hard-confined’ v-groove wires. 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 corresponding Hamiltonian on a finite-difference grid in the z -direction may be written [4]:

$$H = -t \sum_{i,\sigma} \left(c_{i+1,\sigma}^\dagger c_{i,\sigma} + \text{h.c.} \right) + \sum_i \epsilon_i n_i + \frac{1}{2} \sum_{i \neq j} U_{ij} n_i n_j + \frac{1}{2} \sum_{i,\sigma} U_{ii} n_{i,\sigma} n_{i,-\sigma}. \quad (1)$$

This is a general form, the difference between different wire shapes 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 .

In order to study the many-electron problem, it is convenient to express the Hamiltonian in a basis which distinguishes bound and unbound states explicitly. This may be done by first diagonalizing the single-electron part of Eq. (1) with the transformation $c_{q,\sigma} = \sum_i \phi_i^q c_{i,\sigma}$ with eigenenergies ϵ_q . In this basis the Hamiltonian becomes,

$$H = \sum_q \epsilon_q n_q + \frac{1}{2} \sum_{\substack{q_1 q_2 q_3 q_4 \\ \sigma \sigma'}} \mathcal{U}(q_1 q_2 q_3 q_4) c_{q_1,\sigma}^\dagger c_{q_3,\sigma'}^\dagger c_{q_4,\sigma'} c_{q_2,\sigma}, \quad (2)$$

where $\mathcal{U}(q_1 q_2 q_3 q_4) = \sum_{ij} U_{ij} \phi_i^{q_1} (\phi_i^{q_2})^* \phi_j^{q_3} (\phi_j^{q_4})^*$. We further denote the lowest localized state with energy $\epsilon_q < 0$ by $d_\sigma \equiv c_{q,\sigma}$, with $n_d = \sum_\sigma d_\sigma^\dagger d_\sigma$ and, similarly, the scattering states with positive ϵ_q are distinguished by $q \rightarrow k$. There are two independent unbound states corresponding to each k and these are chosen to be plane waves asymptotically, i.e. $\phi_j^k \rightarrow e^{ikj}$ as $j \rightarrow \pm\infty$ and $\epsilon_k = \frac{\hbar^2 k^2}{2m^*}$. Retaining only those Coulomb matrix elements which involve both localized

and scattered electrons, omitting all terms which would give rise to states in which the localized state is unoccupied, we arrive at an Anderson-type Hamiltonian,

$$\begin{aligned}
H = & \sum_k \epsilon_k n_k + \epsilon_d n_d + \sum_{k,\sigma} (V_k n_{d,-\sigma} c_{k,\sigma}^\dagger d_\sigma + \text{h.c.}) + \\
& + U n_{d\uparrow} n_{d\downarrow} + \sum_{kk',\sigma} M_{kk'} n_d c_{k,\sigma}^\dagger c_{k',\sigma} + \sum_{kk'} J_{kk'} \mathbf{S}_d \cdot \mathbf{s}_{kk'}.
\end{aligned} \tag{3}$$

Here $U = \mathcal{U}(dddd)$ is the Hubbard repulsion, $V_k = \mathcal{U}(dddk)$ is mixing term, $M_{kk'} = \mathcal{U}(ddkk') - \frac{1}{2}\mathcal{U}(dkk'd)$ corresponds to scattering of electrons and the direct exchange coupling is $J_{kk'} = 2\mathcal{U}(dkk'd)$. Spin operators in Eq. (4) are defined as $\mathbf{S}_d = \frac{1}{2} \sum_{\sigma\sigma'} d_\sigma^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} d_{\sigma'}$ and $\mathbf{s}_{kk'} = \frac{1}{2} \sum_{\sigma\sigma'} c_{k,\sigma}^\dagger \boldsymbol{\sigma}_{\sigma\sigma'} c_{k',\sigma'}$, where $\boldsymbol{\sigma}_{\sigma\sigma'}$ are the usual Pauli matrices. Although the Hamiltonian, Eq. (4), is similar to the usual Anderson Hamiltonian [5], we stress the important difference that the kd -hybridisation term above arises solely from the Coulomb interaction, whereas in the usual Anderson case it comes primarily from one-electron interactions. These have been completely eliminated above by solving the one-electron problem exactly. The resulting hybridization term contains the factor $n_{-\sigma}$, and hence disappears when the localized orbital is unoccupied. This reflects the fact that an effective double-barrier structure and resonant bound state occurs via Coulomb repulsion only because of the presence of a localized electron.

In Fig. 1 couplings V_k , $M_{kk'}$ and $J_{kk'}$ are shown for a set of wire parameters used in Fig. 3(a) of Ref. [4].

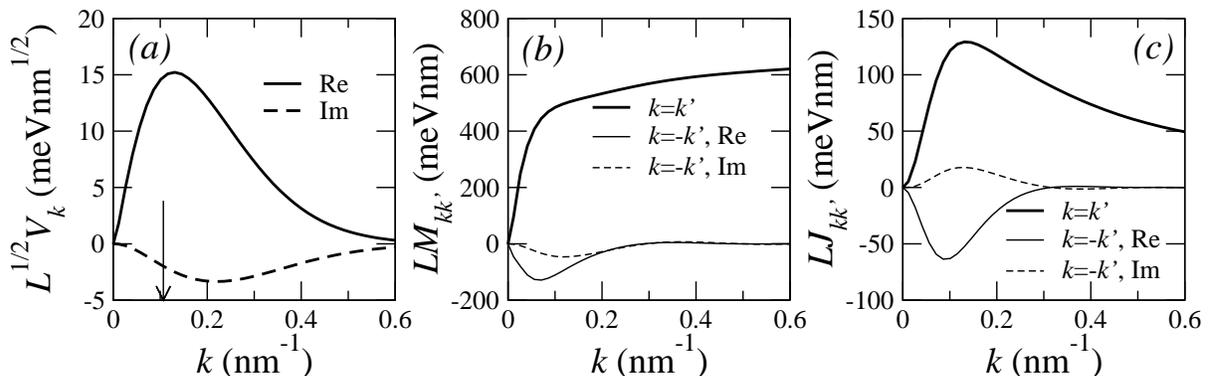


FIG. 1. k -dependence of matrix elements of the effective Anderson model. The wire is parametrised as in Ref. [4] (with $a_0 = 10$ nm, $\xi = 0.24$, $a_1/a_0 = 2$, $V_0 = 0.4$ eV, $\rho = 50$ nm and $\gamma = 1$) (a) Mixing coupling V_k . The energy $\epsilon_d + U$ is indicated with an arrow. (b, c) Scattering couplings $M_{kk'}$ and $J_{kk'}$.

The scattering solutions of the Hamiltonian (4) were obtained exactly for two electrons with the boundary condition that for $z \rightarrow \infty$, one electron occupies the lowest bound state, whilst the other is in a forward propagating plane wave state, $\phi_k(z) \sim e^{ikz}$. From these solutions we compute the conductance using the Landauer-Büttiker formula which, incorporating the results of spin-dependent scattering, takes the following form [4],

$$G(\mu) = \frac{2e^2}{h} \int \frac{-\partial f(\epsilon - \mu, T)}{\partial \epsilon} \left[\frac{1}{4} \mathcal{T}_s(\epsilon) + \frac{3}{4} \mathcal{T}_t(\epsilon) \right] d\epsilon \tag{4}$$

where \mathcal{T}_s and \mathcal{T}_t are the singlet and triplet transmission probabilities respectively and μ is the Fermi energy in the leads. In Fig. 2 \mathcal{T}_s , \mathcal{T}_t and conductance $G(\mu)$ are presented.

The thin lines are the exact scattering result for two electrons. This shows 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. This is a universal effect in one-dimensional systems with very weak longitudinal confinement. The emergence of a specific structure 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. The solid lines show the exact scattering solutions for the Anderson-type Hamiltonian, for which the matrix elements, and their energy dependence are calculated explicitly. The solution of this Anderson-type model for two electrons, in which the localized level always contains at least one electron, reproduce the main features of the exact scattering solutions of the original model. The energy dependence of the matrix elements is essential to get this good agreement. We have also solved a similar model in which plane waves, rather than exact scattering states of the non-interacting problem, were used. However, this gave poor agreement with the exact results. We conclude that an Anderson-type model is adequate for a near-perfect quantum wire provided that a suitable basis set is used and the energy-dependence of

the matrix elements is accurately determined. Future work will focus on the many-electron properties of this effective Hamiltonian, including ‘Kondo’ and ‘mixed valence’ regimes.

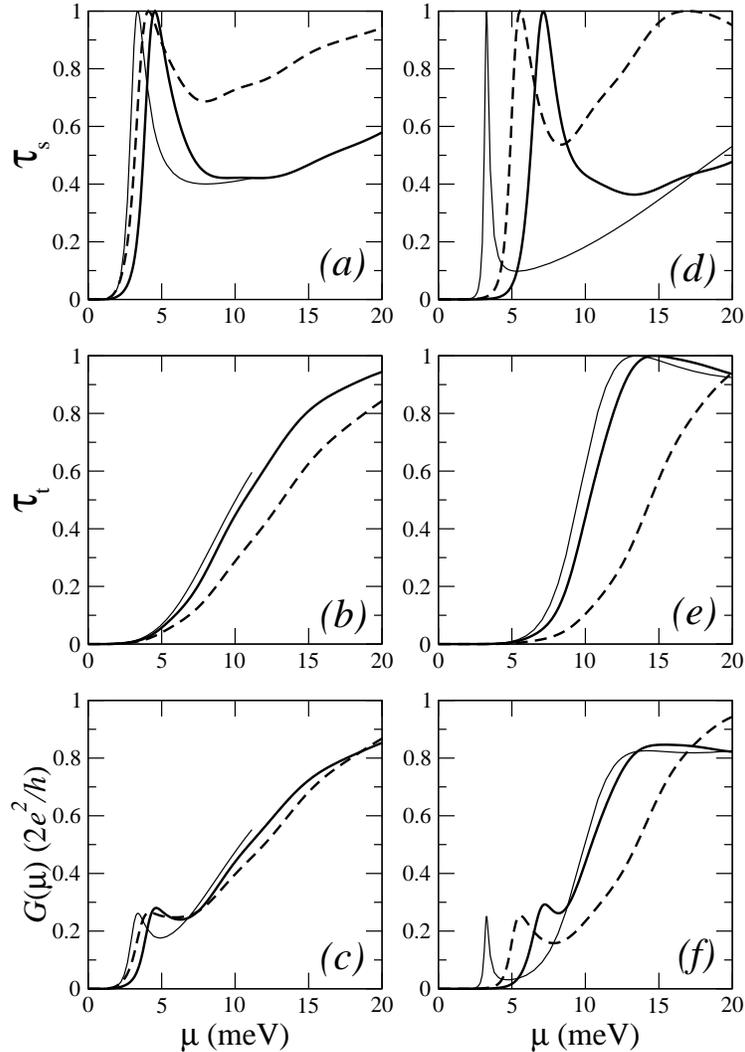


FIG. 2. Singlet (a, d) and triplet (b, e) transmission probabilities and corresponding conductances (c, f). Parameters for the left set are as in Fig. 1, for the right set: $a_0 = 10$ nm, $\xi = 0.15$, $a_1/a_0 = 4$, $V_0 = 0.4$ eV, $\rho = 100$ nm and $\gamma = 0.9$. Thin lines represent exact results from Eq. (1), thick lines are results from Eq. (4). Dashed lines show results where the exchange term in Eq. (4) is neglected.

ACKNOWLEDGMENTS

This work was part-funded by the U.K. Ministry of Defence and the EU.

-
- [1] B.J. van Wees *et al.*, Phys. Rev. Lett. **60**, 848 (1988); D.A. Wharam *et al.*, J. Phys. C **21**, L209 (1988).
[2] A. Yacoby *et al.*, Phys. Rev. Lett. **77**, 4612 (1996); P. Ramvall *et al.*, Appl. Phys. Lett. **71**, 918 (1997); M. Grundmann *et al.*, Semicond. Sci. Tech. **9**, 1939 (1994); R. Rinaldi *et al.*, Phys. Rev. Lett. **73**, 2899 (1994); K.J. Thomas *et al.*, Phys. Rev. Lett. **77**, 135 (1996); Phys. Rev. B **58**, 4846 (1998); D. Kaufman *et al.*, Phys. Rev. B **59**, R10433 (1999); D.J. Reilly, cond-mat/0001174.
[3] R. Landauer, IBM J. Res. Dev. **1**, 223 (1957); **32**, 306 (1988); M. Büttiker, Phys. Rev. Lett. **57**, 1761 (1986).

- [4] T. Rejec, A. Ramšak, and J.H. Jefferson, cond-mat/9910399 (submitted to Phys. Rev. B); T. Rejec, A. Ramšak, and J.H. Jefferson, J. Phys.: Condens. Matter **12**, L233 (2000).
- [5] G.D. Mahan, *Many-Particle Physics*, Plenum Press, New York (1990).