Spin-dependent resonances in the conduction edge of quantum wires

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The conductance through a quantum wire of cylindrical cross section and a weak bulge is determined exactly for two electrons within the Landauer-Büttiker formalism. We show that this ''open'' quantum dot exhibits spin-dependent resonances resulting in two anomalous structure on the rising edge to the first conductance plateau, one near $0.25(2e^2/h)$, related to a singlet resonance, and one near $0.7(2e^2/h)$, related to a triplet resonance. These resonances are generic and robust, occurring for other types of quantum wires and surviving to temperatures of a few degrees.

Recent technological advances have enabled semiconductor quantum wires to be fabricated with effective wire widths down to a few nanometers, for example, by heteroepitaxial growth on v-groove surfaces,[1] epitaxial growth on ridges,[2] cleaved edge overgrowth,[3] etched wires with gating,[4] and gated two-dimensional electron gas (2DEG) structures.[5,6] More recently, there has been considerable interest in carbon nanotubes for which the quantum wire cross section can approach atomic dimensions. Such structures have potential for optoelectronic applications, such as light-emitting diodes, low-threshold lasers and single-electron devices.

Many groups have now observed conductance steps in all of these various types of quantum wire, following the pioneering work in Refs. 5 and 6. While these experiments are broadly consistent with a simple noninteracting picture,[7] there are certain anomalies, some of which are believed to be related to electron-electron interactions and appear to be spin-dependent. In particular, a structure is seen in the rising edge of the conductance curve, starting at around $0.7(2e^2/h)$ and merging with the first conductance plateau with increasing energy.[8] This structure, already visible in the early experiments,[5] can survive to temperatures of a few degrees and also persists under increasing source-drain bias, even when the conductance plateau has disappeared. Under increasing in-plane magnetic field, the structure moves down, eventually merging with the e^2/h conductance plateau at very high fields. Theoretical work has attempted to explain these observation in various ways, including conductance suppression in a Luttinger liquid with repulsive interaction and disorder,[9] local spin-polarized density-functional theory,[10] and spin-polarized subbands.[11] In some of the more recent experiments, an anomaly is seen at lower energy with conductance around $0.2(2e^2/h)$.[12,2] This can also survive to a few degrees though is less robust than the 0.7 anomaly and is more readily suppressed by a magnetic field.[2]

In this paper, we suggest that these anomalies are related to weakly bound states and resonant bound states within the wire. These would arise, for example, if there is a small fluctuation in the thickness of the wire in some region, giving rise to a weak bulge. If this bulge is very weak, then only a single electron will be bound. We may thus regard this system as an ''open'' quantum dot in which the bound electron inhibits the transport of conduction electrons via the Coulomb interaction. Near the conduction threshold, there will be a Coulomb blockade and we show below that this also gives rise to a resonance, analogous to that which occurs in the single-electron transistor.[13] This is a generic effect arising from an electron bound in some region of the wire and such binding may arise from a number of sources, which we do not consider explicitly. For example, in addition to a weak thickness fluctuation, a smooth variation in confining potential due to remote gates, contacts, and depletion regions could contribute to electron confinement along the wire or gated 2DEG. In this paper we consider only very weak confinement near the conductance threshold for which a single electron is bound.

We consider a straight quantum wire with a small fluctuation in thickness giving rise to a weak ''bulge.'' The original motivation behind this work was to examine ballistic transport through wires produced in v grooves, similar to the those reported by Kaufman *et al.*,[12] with mean thicknesses in the range 10–20 nm and small thickness fluctuations. Although the cross section of these wires is crescent shaped, this was approximated to circular for simplicity. We later realized that the precise shape of the cross section is not fundamentally important for the existence of conductance anomalies in the rising edge to the first conductance peak. We have performed detailed calculations for wires of circular cross section and for planar wires and, apart from small quantitative differences, the results are very similar. For brevity we present here the results for wires of circular symmetry about the z axis and with constant potential, $V(r,z)=0$ within a boundary $r_0(z)$ from the symmetry axis and confining potential $V_0>0$ elsewhere. To be definite, we choose parameters appropriate to GaAs for the wire and $Al_xGa_{1-x}As$ for the barrier with x such that $V_0=0.4$ eV, which is close to the crossover to indirect gap. Band nonparabolicity is neglected and we use the GaAs effective mass, $m^*=0.067m_0$, neglecting its variation across the boundary. The wire width is taken as $r_0(z)=\frac{1}{2}a_0(1+\xi\cos^2\pi z/a_1)$ for

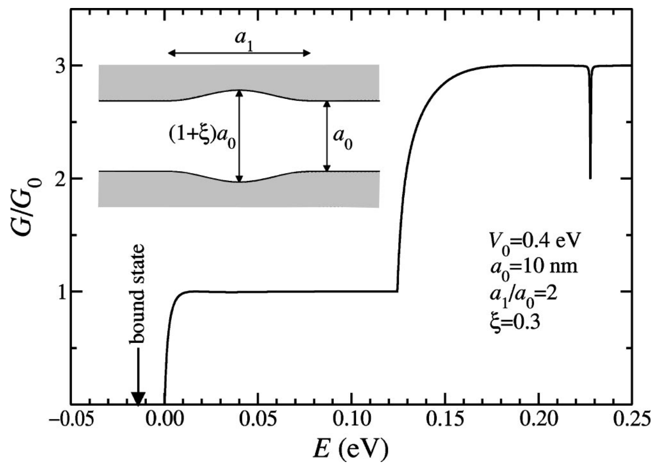

FIG. 1. Conductance G/G_0 for one (noninteracting) electron. The energy E is measured from the bottom of the lowest transverse channel. Inset: geometry of the open quantum dot is determined with $r_0(z)=\frac{1}{2}a_0(1+\xi\cos^2\pi z/a_1)$.

$|z|\leq\frac{1}{2}a_1$ and $r_0(z)\equiv\frac{1}{2}a_0$ otherwise, i.e., a wire of width a_0 with a single bulge of length a_1 and width $(1+\xi)a_0$, as shown in Fig. 1 (inset).

When the wire is connected to metallic source-drain contacts, electrons will flow into the wire region as the Fermi energy is raised from below the conduction band edge via a gate (not considered explicitly). At least one electron will then become bound in the bulge region of the wire. The number of bound electrons depends on both the Fermi energy and the relative size of the bulge (i.e., parameters a_1 and ξ). We first consider the noninteracting electron problem for unbound (scattering) states. As shown in Refs. 14 and 15 for a two-dimensional wire, this problem may be reduced to a quasi-one-dimensional problem by expanding in transverse modes. The one-electron Schrödinger equation,

$$-\frac{\hbar^2}{2m^*}\nabla^2\Psi(x,y,z)+V\Psi(x,y,z)=E\Psi(x,y,z), \qquad (1)$$

then reduces to an N-component differential equation that is solved for the scattering states. The number of channels, N, is chosen to be sufficiently large to give convergence and depends upon the Fermi energy in the leads and the dot parameter ξ. For large ξ many channels are needed since the rapid change in wire thickness gives rise to large interchannel mixing. From the solution of the scattering problem, the conductance is calculated from the usual Landauer-Büttiker formula,[16] $G=G_0\,\mathcal{T}(E)$, where $G_0=2e^2/h$, E is the Fermi energy and $\mathcal{T}(E)$ is the total transmission probability. This is shown in Fig. 1 for a wire with dot parameter $\xi=0.3$. For such a small ξ the conductance is very similar to that of a perfect straight wire, as we would expect, with conductance steps at G_0, $3G_0$, $5G_0$, etc. The main difference is the very sharp Fano antiresonance seen in the second conductance step, a consequence of interchannel mixing, which is washed out at finite temperature. Apart from this resonance, all other features, including the position of a bound state below the conduction edge, may be accurately described by neglecting coupling between channels. With such weak confinement, there is only one bound state.

We now consider the interacting electron problem with wire thickness variation in a range that ensures that only one electron occupies a bound state and that restriction to a single channel near the conduction edge is an excellent approximation. To determine the conductance of this system in the ballistic regime we need to solve the two-electron scattering problem at low energy, for which one electron always remains bound for ingoing and outgoing states. To do this we start with the single-channel, two-electron Schrödinger equation for electron motion in the z direction,

$$\left[-\frac{\hbar^2}{2m^*}\left(\frac{d^2}{dz_1^2}+\frac{d^2}{dz_2^2}\right)+\epsilon(z_1)+\epsilon(z_2)\right]\psi(z_1,z_2)$$
$$+U(z_1,z_2)\psi(z_1,z_2)=E\psi(z_1,z_2), \qquad (2)$$

where $\epsilon(z)$ is the energy of the lowest transverse channel at z and $U(z_1,z_2)$ is the effective two-electron interaction given by integrating the full three-dimensional (3D) unscreened Coulomb interaction over the lowest transverse mode. Although this equation is exact for the two-electron problem within the single-channel approximation, we add a phenomenological screening factor to the two-electron interaction term to mimic the effect of screening by other conduction electrons not accounted for explicitly. The two-electron interaction then has the form $U(z_1,z_2)=e^2/[4\pi\varepsilon\varepsilon_0 d(z_1,z_2)]\exp(-|z_1-z_2|/\rho)$, with $d(z_1,z_2)\rightarrow|z_1-z_2|$ for large d. The dielectric constant is taken as $\varepsilon=12.5$, appropriate for GaAs.

We see that Eq. (2) has a rather general form that can arise in a variety of different circumstances. The transverse one-electron energy, $\epsilon(z)$, arising from the weak bulge in the wire, is equivalent to a shallow one-electron potential energy in the z direction and arises for wires of any cross section (circular, planar, crescent-shaped, etc.). Such a potential also arises in perfectly straight wires subject to smooth, weak potential variations from remote charge distributions, image charge in remote gates, etc. Hence, although the Hamiltonian equation (2) was derived for a certain type of quantum wire, it is actually applicable to a much wider class of wires and ''open dot'' systems, physically different cases merely modifying the effective one-electron energies $\epsilon(z)$, the length parameter $d(z_1,z_2)$ and the screening length ρ. The only restriction is that the deviation from a perfectly straight wire be sufficiently small, since this ensures the validity of the lowest channel approximation and the problem becomes essentially one-dimensional. There will, of course, be quantitative differences in different situations but, provided the effective potential has a weak minimum, then it will give rise to conductance anomalies similar to those that we discuss below. In this sense the model is generic.

If we discretize Eq. (2) by the usual method of finite differences, then the Hamiltonian may be mapped onto an extended Hubbard model with effective Hamiltonian,

$$H=-t\sum_{i\sigma}\left(c^\dagger_{i+1,\sigma}c_{i\sigma}+c^\dagger_{i\sigma}c_{i+1\sigma}\right)+\sum_i\epsilon_i n_i$$
$$+\sum_i U_{ii}n_{i\uparrow}n_{i\downarrow}+\frac{1}{2}\sum_{i\neq j}U_{ij}n_i n_j, \qquad (3)$$

where $c_{i\sigma}^{\dagger}$ creates an electron with spin σ at $z=z_i$ in the lowest transverse channel; $n_i=\Sigma_\sigma n_{i\sigma}$ with $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$, $t=\hbar^2/(2m^*\Delta^2)$, where $\Delta=z_{i+1}-z_i$, $\epsilon_i=\hbar^2/(m^*\Delta^2)+\epsilon(z_i)$, and $U_{ij}=U(z_i,z_j)$. This mapping is exact in the limit $\Delta\rightarrow 0$ for which Eq. (3) becomes the real-space field-theory representation of the Hamiltonian in Eq. (2). In all calculations, we have chosen Δ to be sufficiently small to ensure convergence.

We now consider the interacting two-electron scattering problem in which the initial ''ingoing'' state consists of one electron bound in the quantum dot region, with energy E_0, and the other electron far away from this bound electron but with kinetic energy (Fermi energy ϵ_F in the lead) sufficiently small that all possible outgoing states also have an electron bound in the dot region. This is elastic scattering, satisfied when $\epsilon_F+E_0<0$, which is the case of interest, close to the conduction edge. The problem considered here is analogous to treating the collision of an electron with a hydrogen atom as, e.g., in Ref. 17. It should be noted that the existence of a single-electron bound state is guaranteed in one dimension, for wells in the z direction, and in this sense is a universal feature. With the chosen parameter range, a second electron cannot be bound due to Coulomb repulsion.

We solve the two-electron problem exactly for this case of elastic scattering, subject to the conditions that the exact ''orbital'' wave functions must be either symmetric (singlet) or antisymmetric (triplet). The solutions for the transmission amplitudes are obtained by solving a set of linear equations. From these solutions we compute conductance using the Landauer-Büttiker formula, generalized to incorporate the symmetric and antisymmetric nature of the states. The Landauer-Büttiker formula then takes the following form in zero magnetic field,

$$G=G_0\left[\frac{1}{4}\mathcal{T}_s(E)+\frac{3}{4}\mathcal{T}_t(E)\right], \tag{4}$$

where the subscripts s and t refer to singlet and triplet configurations, respectively. This formula is justified (and exact) for the case of elastic scattering, which is the regime of interest for this paper. At energies high enough that the scattered electron could excite the bound electron in the continuum, a more general treatment would be required.[18]

In Fig. 2 we show plots at zero temperature of $\mathcal{T}_s(E)$, $\mathcal{T}_t(E)$, and G/G_0 for a typical wire of width $a_0=10$ nm, dot width $(1+\xi)a_0=11.1$ nm, dot length $a_1=50$ nm, and screening lengths of 25 nm, 50 nm, and infinity. Similar results are obtained for thicker wires, up to $a_0\sim 50$ nm, beyond which the single-channel approximation becomes less reliable as electron correlations become increasingly important. Note that for weak coupling, the energy scale is set by the position of the lowest channel, $\sim 1/a_0^2$, and hence the conductance versus Ea_0^2 is roughly independent of a_0.

The main feature of these results is that there are resonances in both singlet and triplet channels and these give rise to structures in the rising edge to the first conductance plateau for $G\sim\frac{1}{4}G_0$ (singlet) and $G\sim\frac{3}{4}G_0$ (triplet). Furthermore, as the screening is increased (screening length reduced) we see that these resonances shift to lower energy. This behavior has the following simple interpretation. The incident electron ''feels'' the Coulomb potential of the elec-

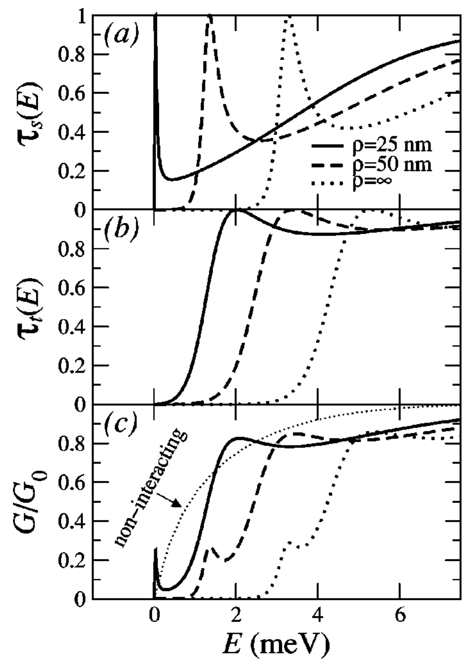

FIG. 2. (a) Zero temperature singlet (elastic) transmission probability $\mathcal{T}_s(E)$ and (b) triplet $\mathcal{T}_t(E)$ for various screening lengths ρ. The energy E is defined as in Fig. 1. (c) Total conductance, $G/G_0=\frac{1}{4}\mathcal{T}_s(E)+\frac{3}{4}\mathcal{T}_t(E)$. Thin dotted line represents the corresponding noninteracting result.

tron bound in the dot region and there is thus a gradual increase in conductance with energy, the threshold shifting to lower energies as the screening is increased. The resonances occur because the potential ''felt'' by the incident electron passes through a minimum at the center of the dot, where the transverse channel energy is lowest. Thus, the incident electron ''sees'' a double barrier, which will have some resonant energy for which there is perfect transmission. A more detailed analysis has to account for spin, and this may be understood by gradually switching on the Coulomb interaction. For the present choice of parameters, and also a range of parameter sets that correspond to a very weak bulge, there are two bound states for one electron. With no interaction both electrons may thus occupy one of four states (three singlets and a triplet). If we now switch on a small Coulomb interaction, then the lowest two-electron state will be a singlet, derived from both electrons in the lowest one-electron state. We may regard one electron as occupying the lowest bound-state level and the other electron of opposite spin also in this same orbital state but for energy U higher, where U is the intra-atomic Coulomb matrix element, as in the Anderson impurity model.[19] As the Coulomb interaction is increased, U eventually exceeds the binding energy and this higher level becomes a virtual bound state, giving rise to a resonance in transmission. An estimate of the energy of the virtual bound state is given by the Anderson Coulomb matrix element with both electrons in the one-electron orbital ψ_0, i.e., $U=\int dz\,dz'|\psi_0(z)|^2|\psi_0(z')|^2U(z,z')$. We have computed this and get reasonable agreement with the exact result.

We can, in addition, approximate the full scattering problem by solving the Hartree-Fock equations without iteration in which one of the electrons again occupies ψ_0. The agree-

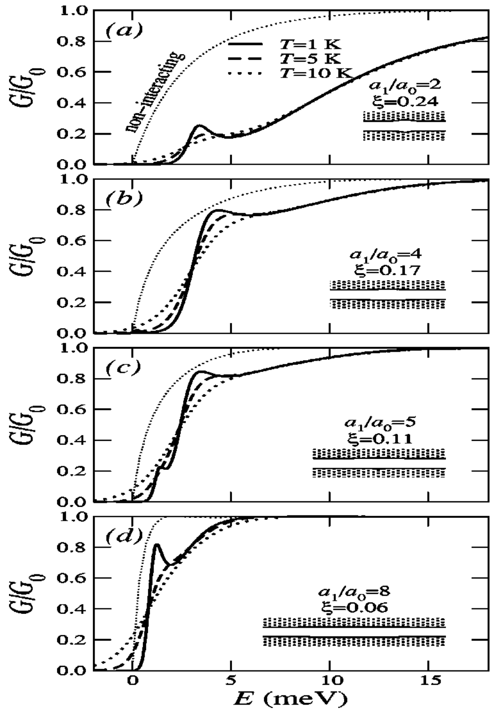

FIG. 3. Conductance G/G_0 for various shapes of the dot and for various temperatures, with screening length $\rho=50$ nm.

ment is also very good and reproduces all the resonance features. When both electrons have the same spin then they must occupy different orbitals in the dot region when the Coulomb interaction is switched off. With small Coulomb interaction the resulting triplet is the lowest two-electron excited state, and this develops into a resonant bound state with the full Coulomb interaction, with energy at approximately $E_1+U_1-J_1$, where E_1 is the energy of the second one-electron state with U_1 and J_1 the respective Coulomb and exchange integrals. The next excited (singlet) resonant bound state is $2J_1$ higher in energy, which is into the first conductance plateau region where it has little effect. We see from Fig. 2 that the singlet resonance is somewhat sharper than the triplet and this is simply because it is lower in energy and closer to a ''real'' bound state.

The resonances have a strong temperature dependence and, in particular, the sharper singlet resonance is more readily eliminated at finite temperatures. This can be seen in Fig. 3 where we have plotted the conductance calculated using a generalized Landauer formula[20,15] at $T=1$, 5, and 10 K for wires in which the bulge region is becoming progressively longer and flatter, i.e., approaching a perfectly straight wire. In Fig. 3(a), with the most pronounced deviation from a straight wire, there is only one single-electron bound state, and hence only one resonant bound state, giving rise to a peak in the conductance with $G\sim 0.3G_0$ at 1 K, developing into a step at 5 K, and gradually disappearing for $T>10$ K. This behavior is expected for hard-confined wires, such as those produced in v grooves, where smooth fluctuations in thickness of this order would be reasonable and, indeed, similar behavior has been recently observed.[12] In Fig. 3(b) the $T=0$ singlet resonance is so sharp that even at 1 K it has already disappeared, and we see only the triplet resonance, which is quite pronounced and develops into a step as the temperature is increased, being still quite discernible at 10 K. As we progress to a straighter wire in Fig. 3(c) we can resolve the singlet step at 1 K, but this is readily damped out as the temperature is increased and finally for the straightest wire in Fig. 3(d), the singlet is again unresolvable but is now engulfed by the triplet resonance, which is very close in energy.

These results are consistent with experiments on gated quantum wires and show that only a very small deviation from a perfectly straight wire with constant potential can give rise to the reported steplike features near $G=0.7(2e^2/h)$. Furthermore, our model is consistent with the experimental observations that these steplike anomalies will move towards a plateau at e^2/h as the magnetic field is increased. Further experimental observations on gated wires[8,21] show that as the source-drain bias is increased from zero, an anomaly appears at $G\sim 0.25(2e^2/h)$, coexisting with the $0.7(2e^2/h)$ anomaly. This sharpens as the bias is increased and, in the example of Ref. 21, for $V_{sd}\sim 6$ mV the 0.25 anomaly is very pronounced whilst the 0.7 anomaly has disappeared. This is also consistent with the above model since under bias the triplet resonant bound state will eventually disappear because the confining potential in the z direction will only accommodate a single one-electron bound state, giving rise to a singlet resonance only. Furthermore, this resonance will become broader with increasing bias, resulting in a more pronounced step, as observed. Whilst the gross features of many of the observed results may be interpreted in terms of this simple model of spin-dependent scattering from a single-bound electron, the observation of anomalies in a wide variety of samples would mitigate against the shallow longitudinal confinement potential as always arising from thickness fluctuations or depletion charge. We suggest further experimental study of this effect.

In conclusion, we have shown that quantum wires with weak longitudinal confinement can give rise to spin-dependent resonances when a single electron is bound in the confined region, a universal effect in one-dimensional systems with very weak longitudinal confinement. The positions of the resulting features at $G\sim\frac{1}{4}G_0$ and $G\sim\frac{3}{4}G_0$ are a consequence of the singlet and triplet nature of the resonances. These resonances have their origin in the repulsive Coulomb interaction between the electrons, coupled with the effective one-electron potential well. This results in an effective double barrier for one electron due to the Coulomb repulsion of the other and in this sense is analogous to Coulomb blockade resonances in quantum dots. The behavior of the two systems is similar in the sense that at low energy, conductance is blocked in both cases due to Coulomb repulsion (blockade regime) and increases to a maximum at the resonance energy. At higher energy, beyond the maximum, the current reduces in both cases but this effect is less pronounced in the case of the wire since the effective barriers become weak at high energy and the resonance peaks develop into shoulders as the temperature is raised. However, in the region of the resonances at low temperatures, the physics of the conductance is essentially the same in both cases, with the charge fluctuating between one and two electrons on resonance. There are also strong spin effects in both cases, though for large quantum dots the Coulomb repulsion effects dominate and the small spin splitting between singlet and triplet resonances (in the case of charge fluctuations between one and two electrons) may not be resolved. The competition between attractive one-electron interaction and Coulomb repulsion between two electrons has also been considered recently from a different point of view.[22] This work shows that the effective Coulomb interaction is renormalized and this can also lead to resonant transmission of the two electrons.

It should be noted that the existence of a single-electron bound state is guaranteed in one-dimensional systems with the geometry studied here. The emergence of a specific structure at $G(E)$ as 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. Our comprehensive numerical investigation of open quantum dots using a wide range of parameters (for a circular and rectangular[23] cross section of the wire) shows that singlet resonances are always at lower energies than the triplets, in accordance with the Lieb-Mattis theorem for bound states[24] and in contrast to the proposed scenario of Flambaum and Kuchiev,[25] where the interaction would be attractive and the triplet would be the lowest state. Further experiments in which the widths of quantum wires and/or the confinement potentials are engineered to control longitudinal confinement should throw further light on the problem of spin-dependent ballistic transport.

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