Kondo Model for the "0.7 Anomaly" in Transport through a Quantum Point Contact

Yigal Meir,^{1,2,*} Kenji Hirose,³ and Ned S. Wingreen¹

¹NEC Research Institute, 4 Independence Way, Princeton, New Jersey 08540

²Physics Department, Princeton University, Princeton, New Jersey 08540

³Fundamental Research Laboratories, NEC Corporation, 34 Miyukigaoka, Tsukuba, Ibaraki 305-8501, Japan

(Received 1 July 2002; published 21 October 2002)

Experiments on quantum point contacts have highlighted an anomalous conductance plateau around $0.7(2e^2/h)$, with features suggestive of the Kondo effect. Here, an Anderson model for transport through a point contact analyzed in the Kondo limit. Hybridization to the band increases abruptly with energy but decreases with valence, so that the background conductance and the Kondo temperature T_K are dominated by different valence transitions. This accounts for the high residual conductance above T_K . The model explains the observed gate-voltage, temperature, magnetic field, and bias-voltage dependences. A spin-polarized current is predicted even for low magnetic fields.

DOI: 10.1103/PhysRevLett.89.196802

PACS numbers: 73.61.-r, 71.15.Mb, 71.70.Ej, 75.75.+a

The conductance through quantum point contacts (QPCs) is observed to be quantized in units of $2e^2/h$ [1,2]. In addition to these integer conductance steps, an extra conductance plateau around $0.7(2e^2/h)$ has attracted considerable experimental effort [3–6] and drawn attention to the effects of electron-electron interaction on the transport properties of low-dimensional quantum systems [7–10]. A recent experiment [11] has highlighted features in QPC transport strongly suggestive of the Kondo effect: a zero-bias peak in the differential conductance which splits in a magnetic field, and a crossover to perfect transmission below a characteristic "Kondo" temperature T_K , consistent with the peak width. A puzzling observation was the large value of the residual conductance, $G > 0.5(2e^2/h)$, for $T \gg T_K$.

Here we demonstrate the applicability of an Anderson model to transport through a QPC by comparing the results of perturbation theory in the Kondo limit to experimental data. A novel feature in the model distinguishes transport through a QPC from transport through other Kondo impurities, e.g., quantum dots [12], and explains the large residual conductance: the hybridization to the band is a strong function of energy and valence. Predictions of the model include binding of an electron at the QPC *before* the first conductance step, and a strongly spin-polarized current at magnetic fields satisfying $g^* \mu_B B > k_B T_K$, $k_B T$.

Use of an Anderson model for a QPC is motivated below by spin-density-functional-theory results indicating that a single electron can bind at the center of the QPC. An intuitive picture is to consider transport across a square barrier. For a wide and tall barrier, in addition to the exponentially increasing transparency, there are narrow transmission resonances above the barrier. These result from multiple reflections from the edges of the barrier, and are associated with quasibound states, which can play the role of localized orbitals in an Anderson model. Our SDFT results indicate that even an initially smooth QPC potential can produce a narrow quasibound state, resulting in a spin bound at the center of the QPC. We thus model the QPC and its leads by an Anderson Hamiltonian [13]

$$H = \sum_{\sigma;k\in L,R} \varepsilon_{k\sigma} \mathbf{c}_{k\sigma}^{\dagger} \mathbf{c}_{k\sigma} + \sum_{\sigma} \varepsilon_{\sigma} \mathbf{d}_{\sigma}^{\dagger} \mathbf{d}_{\sigma} + U \mathbf{n}_{\dagger} \mathbf{n}_{\downarrow} + \sum_{\sigma;k\in L,R} [V_{k\sigma}^{(1)}(1 - \mathbf{n}_{\bar{\sigma}}) \mathbf{c}_{k\sigma}^{\dagger} \mathbf{d}_{\sigma} + V_{k\sigma}^{(2)} \mathbf{n}_{\bar{\sigma}} \mathbf{c}_{k\sigma}^{\dagger} \mathbf{d}_{\sigma} + \text{H.c.}],$$
(1)

where $\mathbf{c}_{k\sigma}^{\dagger}(\mathbf{c}_{k\sigma})$ creates (destroys) an electron with momentum k and spin σ in lead L or R, $\mathbf{d}_{\sigma}^{\dagger}(\mathbf{d}_{\sigma})$ creates (destroys) a spin- σ electron on "the site," i.e., the quasibound state at the center of the QPC, and $\mathbf{n}_{\sigma} = \mathbf{d}_{\sigma}^{\dagger}\mathbf{d}_{\sigma}$. The hybridization matrix elements, $V_{k\sigma}^{(1)}$ for transitions between 0 and 1 electrons on the site and $V_{k\sigma}^{(2)}$ for transitions between 1 and 2 electrons, are taken to be steplike functions of energy, mimicking the exponentially increasing transparency (the position of the step defines our zero of energy). Physically, we expect $V_{k\sigma}^{(2)} < V_{k\sigma}^{(1)}$, as the Coulomb potential of an electron already occupying the QPC will reduce the tunneling rate of a second electron through the bound state. In the absence of magnetic field the two spin directions are degenerate, $\varepsilon_{\downarrow} = \varepsilon_{\uparrow} = \varepsilon_{0}$.

For a noninteracting system, the conductance *G* will be a (temperature broadened) resonance of Lorentzian form, with a width proportional to V^2 . If *V* rises abruptly to a large value, such that the width becomes larger than $\varepsilon_F - \varepsilon_0$, where ε_F is the Fermi energy, *G* saturates to a value of $2e^2/h$. For the interacting system, we similarly expect the *high-temperature* contribution from the $0 \leftrightarrow 1$ valence fluctuations to *G* to saturate at $0.5(2e^2/h)$ for $\varepsilon_F > 0 > \varepsilon_0$, because the probability of an opposite spin electron occupying the site in this regime is ≈ 0.5 . Since $V_{k\sigma}^{(2)}$ may be significantly smaller than $V_{k\sigma}^{(1)}$, the contribution to the conductance from the $1 \leftrightarrow 2$ valence fluctuations may be small, until $\varepsilon_F \simeq \varepsilon_0 + U$. However, the Kondo effect will J

enhance this contribution with decreasing temperature, until at zero temperature the conductance will be equal to $2e^2/h$, due to the Friedel sum rule [14].

To obtain a quantitative estimate of the conductance we note that the relevant gate-voltage range corresponds to the Kondo regime (singly occupied site), a fact further supported by the observation of a zero-bias peak where the conductance first becomes measurable [11], so the Kondo limit of the Anderson Hamiltonian should be applicable. We therefore perform a Schrieffer-Wolff transformation [15] to obtain the Kondo Hamiltonian [16,17]

$$H = \sum_{\sigma;k\in L,R} \varepsilon_{k\sigma} \mathbf{c}^{\dagger}_{k\sigma} \mathbf{c}_{k\sigma} + \sum_{\sigma,\sigma';k,k'\in L,R} [J^{(1)}_{kk'\sigma\sigma} - J^{(2)}_{kk'\sigma\sigma}] \mathbf{c}^{\dagger}_{k\sigma} \mathbf{c}_{k'\sigma} + 2 \sum_{\sigma,\sigma',\alpha,\alpha';k,k'\in L,R} [J^{(1)}_{kk'\sigma\bar{\sigma}} + J^{(2)}_{kk'\sigma\bar{\sigma}}] [\mathbf{c}^{\dagger}_{k\sigma} \vec{\sigma}_{\sigma\sigma'} c_{k'\sigma'}] \cdot \vec{S};$$

$$I^{(i)}_{kk'\sigma\sigma'} = \frac{(-)^{i+1}}{4} \left[\frac{V^{(i)}_{k\sigma} V^{*(i)}_{k'\sigma'}}{\varepsilon_{k\sigma} - \varepsilon^{(i)}_{\sigma}} + \frac{V^{(i)}_{k\sigma} V^{*(i)}_{k'\sigma'}}{\varepsilon_{k'\sigma'} - \varepsilon^{(i)}_{\sigma'}} \right], \qquad (2)$$

where $\varepsilon_{\sigma}^{(1)} = \varepsilon_{\sigma}$ and $\varepsilon_{\sigma}^{(2)} = \varepsilon_{\sigma} + U$. The Pauli spin matrices are indicated by $\vec{\sigma}$, and the local spin due to the bound state is $\vec{S} = \frac{1}{2} \mathbf{d}_{\alpha}^{\dagger} \vec{\sigma}_{\alpha \alpha'} \mathbf{d}_{\alpha'}$.

Following Appelbaum [18], we treat the above Kondo Hamiltonian perturbatively in the couplings $J_{kk'\sigma\sigma'}^{(i)}$. The differential conductance to lowest order, J^2 , is given by

$$G_2 = \frac{4\pi e^2}{\hbar} \rho_L(\varepsilon_F) \rho_R(\varepsilon_F) \Big\{ (J_{LR}^{(-)})^2 + (J_{LR}^{(+)})^2 \times \Big[3 + 2\langle M \rangle \Big(\tanh \frac{\Delta + eV}{2k_BT} + \tanh \frac{\Delta - eV}{2k_BT} \Big) \Big] \Big\},\tag{3}$$

where, for simplicity, $J_{kk'\sigma\sigma'}^{(i)}$ are replaced by their (magnetic-field independent) values at the Fermi energy

$$J_{l\,l'}^{(i)} \equiv J_{k_F \in lk_F \in l'\sigma\sigma}^{(i)} = \frac{(-)^{i+1}V_i^2}{2(\varepsilon_F - \varepsilon_0^{(i)})} f_{\rm FD}(-\varepsilon_F/\delta), \quad (4)$$

where symmetric leads have been assumed, and the V_i and δ are constants. The $J^{(i)}$ increase in a step of the Fermi-Dirac form $f_{\rm FD}(x) = 1/[1 + \exp(x)]$. We define the combinations $J_{ll'}^{(\pm)} = J_{ll'}^{(1)} \pm J_{ll'}^{(2)}$ for, respectively, the direct and exchange couplings in Eq. (2). In (3), $\Delta = g^* \mu_B B$ is the Zeeman splitting, $\langle M \rangle = -(1/2) \tanh(\Delta/2k_B T)$ is the magnetization for the uncoupled site, and $\rho_{L/R}(\varepsilon) =$ $\sum_{k \in L/R} \delta(\varepsilon - \varepsilon_{k\sigma})$ is the single-spin electron density of states in the leads. We assume $\rho = \rho_L(\varepsilon) = \rho_R(\varepsilon)$.

At low temperatures the Kondo effect leads to a logarithmically diverging contribution G_3 (cf. [23]) to the differential conductance at order J^3 [16], due to integrals running from the Fermi energy to either band edge. Because of the steplike increase of the $J^{(i)}$, the band integral for $J^{(1)}$ runs down from ε_F to the hybridization step at zero, but runs up from ε_F to $\varepsilon_0 + U$ for $J^{(2)}$. Since in the region of interest $\varepsilon_0 + U - \varepsilon_F \gg \varepsilon_F$, the logarithmic contribution from $J^{(2)}$ dominates G_3 .

Figure 1 depicts the linear-response conductance $(G_2 + G_3)$. Since G_2 depends only on the values of $J_{LR}^{(i)}$ at ε_F , it is dominated by $J^{(1)}$, while the Kondo enhancement is dominated by $J^{(2)}$. As argued above, the contribution due to $J^{(1)}$ is set around $0.5(2e^2/h)$ by construction, while the contribution due to $J^{(2)}$, resulting from the $1 \leftrightarrow 2$ valence fluctuations is small at high temperature, but grows with decreasing temperature in a form following the Kondo scaling function, $F(T/T_K)$, where $T_K \simeq U \exp[-1/4\rho J^{(2)}) = U \exp[(\varepsilon_F - \varepsilon_0 - U]/2\rho V_2^2]$, in agreement with the experimental observation of a Kondo temperature increasing exponentially with gate

voltage $\sim \varepsilon_F$. Note that in perturbation theory the conductance is not bound by its physical limit: $2e^2/h$.

The dependence of conductance on magnetic field is shown in Fig. 1(b). The Kondo logarithms in G_3 are suppressed, leading to the evolution of the 0.7 plateau towards and below 0.5. In agreement with experiment [11], the conductance is no longer monotonically increasing with Fermi energy ε_F : the energy denominator causes the $J^{(1)}$ contribution to G_2 to decrease, and this is no longer compensated by an increase of G_3 . Because of shortcomings of perturbation theory the conductance at large magnetic field reduces to a value smaller than $0.5(2e^2/h)$.

Figure 2(a) shows the differential conductance as a function of bias voltage, for several values of ε_F and temperatures. Even at the lowest conductances (small ε_F) there is a clear Kondo peak, as is seen in experiment (inset). Because of the suppression of the Kondo effect by voltage, the large voltage traces are independent of temperature, again in agreement with experiment. Magnetic field splits the Kondo peak as shown in Fig. 2(b).

An important prediction of the Kondo model is that the current through a QPC will be spin polarized if the Zeeman splitting is larger than both k_BT and k_BT_K [Fig. 2(c)]. The net spin conductance G_{σ} , is given, to second order in J, by

$$G_{\sigma} = \frac{16\pi e^2}{\hbar} \rho^2 \langle M \rangle [(J_{LR}^{(1)})^2 - (J_{LR}^{(2)})^2].$$
 (5)

Therefore, at low temperatures and in the vicinity of the $0.7(2e^2/h)$ plateau where T_K is small, a QPC can be an effective spin filter.

Last, we present evidence from spin-density-functional theory (SDFT) [19] for the formation of a local moment (bound spin) at the center of a GaAs QPC, which supports

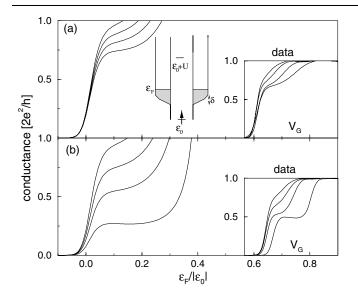


FIG. 1. Results of the Kondo model. (a) Conductance at temperatures T = 0.05, 0.1, 0.2, 0.6 (solid curves, from high to low) as a function of Fermi energy ε_F (all energies in units of $|\varepsilon_0|$). The parameters are $U = 1.45, \rho V_1^2 = 0.12, \rho V_2^2 = 0.015$, and $\delta = 0.02$. Right inset: experimental conductance of QPC at four different temperatures [11]. Center inset: Schematic of the band structure for our Anderson model. (b) Conductance in a magnetic field, for Zeeman splitting $\Delta = 0, 0.07, 0.12, 0.4$ at T = 0.06 (solid curves from top to bottom). Inset: experimental conductance of QPC at different magnetic fields [11].

our use of the Anderson model. SDFT is applied within the local-density approximation [20,21]. The external potential consists of a clean quantum wire with a parabolic confining potential of $V_{\text{wire}}^0(y) = (1/2)m^*\omega_y^2 y^2$ and a QPC potential

$$V_{\text{OPC}}(x, y) = V(x)/2 + m^* [V(x)/\hbar]^2 y^2/2,$$
 (6)

where $V(x) = V_0/\cosh^2(\alpha x)$, with $\alpha = \omega_x \sqrt{m^*/2V_0}$. A contour plot of the QPC potential $V_{\text{QPC}}(x, y)$ is shown in the left inset of Fig. 3(b).

We solve the Kohn-Sham equation [20] using the material constants for GaAs, $m^* = 0.067m_0$ and $\kappa = 13.1$. The external confinement in the y direction in the wire is fixed by $\hbar \omega_y = 2.0$ meV. The parameters for the QPC potential are taken to be $V_0 = 3.0$ meV and $\hbar \omega_x = 1.5$ meV.

Figure 3(a) shows the spin-dependent, self-consistent QPC barriers at T = 0.1 K obtained from SDFT [22]. The local density of states $\nu(\epsilon)$ at the center of the QPC is shown for both spin-up and spin-down in the right inset. Figure 3(b) shows the average 1D electron density through the QPC and the net density of spin-up electrons. The integrated spin-up density is 0.96 electrons. The data from SDFT gives strong evidence for a quasibound state centered at the QPC: there is a resonance in the local density of states $\nu(\epsilon)$ for spin-up, with a net of one spin

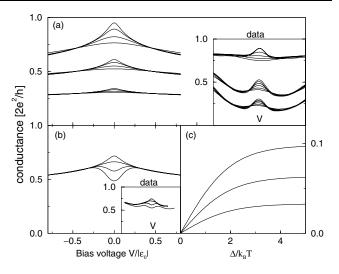


FIG. 2. Differential conductance dI/dV for the Kondo model. (a) dI/dV versus bias at Fermi energies $\varepsilon_F = 0.1, 0.03, 0.01$ from the top group to the bottom. For each chemical potential curves are shown for temperatures T = 0.06, 0.1, 0.2, 0.4 from top to bottom. All other parameters are the same as in Fig. 1. Inset: experimental differential conductance [11]. (b) dI/dV in magnetic fields with Zeeman splitting $\Delta = 0, 0.04, 0.07, 0.1$ at T = 0.06, and $\mu = 0.04$. Inset: experimental differential conductance $d(I_1 - I_1)/dV$ as a function of magnetic fields, for several values of ε_F .

bound in the vicinity of the QPC. The transmission coefficient $T(\epsilon)$ for electrons in the lowest subband is shown in the left inset to Fig. 3(a). Transmission for spin-up is approximately one over a broad range of energies above the spin-up resonance. This implies an onset of strong hybridization at energies above the quasibound state. As the external QPC barrier becomes flatter in the x direction, the width of the quasibound state, and consequently the Kondo temperature, decrease [22], consistent with experimental observations that the "0.7 plateau" decreases towards 0.5 with increasing QPC length.

We have presented a microscopic Anderson model, supported by spin-density-functional theory, for transport through a quantum point contact. The anomalous $0.7(2e^2/h)$ plateau is attributed to a high background conductance plus a Kondo enhancement. The temperature scales for these two contributions are decoupled: $0 \leftrightarrow 1$ valence transitions account for the background conductance, while $1 \leftrightarrow 2$ valence transitions give the dominant Kondo effect. Based on this model one can make specific experimental predictions. A strongly spin-polarized current is predicted when the Zeeman splitting exceeds both k_BT and k_BT_K . The predicted formation of a bound state (local moment) can be directly tested by measuring transport through two parallel point contacts, coupled capacitively, with one of them tuned to $G \simeq e^2/h$, i.e., in the region of maximal sensitivity to its environment. When the gate voltage controlling the other point contact

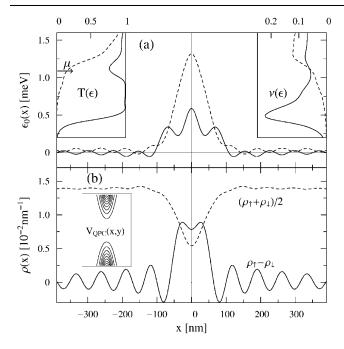


FIG. 3. Results of spin-density-functional theory. (a) Selfconsistent "barrier," i.e., energy of the bottom of the lowest 1D subband at temperature T = 0.1 K as a function of position x in the direction of current flow through the QPC. The electrochemical potential μ is indicated by an arrow on the left. In this panel, solid curves are for spin-up electrons and dashed curves are for spin-down electrons. Left inset: transmission coefficient. Right inset: local density of states at center of QPC. (b) 1D electron density in QPC. The solid curve gives the net spin-up density, and the dashed curve gives the spinaveraged density. Inset: contour plot of the QPC potential $V_{\text{QPC}}(x, y)$.

is scanned through the electron binding event (predicted to occur for $G \ll e^2/h$), an abrupt decrease should be seen in the conductance of the half-transparent point contact. (A very similar arrangement was used recently to probe the bound states of a quantum dot [23].) The presence of bound spins in QPCs near pinchoff has potentially profound effects on transport through quantum dots with QPCs as leads. In particular, the leads may act as magnetic impurities, and cause the apparent saturation of the dephasing time in transport through open semiconductor quantum dots at low temperatures [24], and may complicate attempts to measure the spin of dot electrons [25].

The calculations presented in this paper were perturbative and thus the comparison with experiment could be only semiquantitative. The main failure of perturbation theory is its inability to obtain the low-temperature unitarity limit $2e^2/h$. We hope that our work will motivate more accurate treatments of the Anderson and Kondo models introduced here.

We acknowledge fruitful discussions with B. Altshuler, D. Goldhaber-Gordon, B. Halperin, C. Marcus, and

M. Pustilnik. Y. M. acknowledges partial support by BSF, by NSF Grant No. DMR 00-93079 and by DOE Grant No. DE-FG02-00ER45790.

- *Permanent Address: Department of Physics, Ben-Gurion University, Beer Sheva 84105, Israel.
- [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] K. J. Thomas *et al.*, Phys. Rev. Lett. **77**, 135 (1996); Phys. Rev. B **58**, 4846 (1998).
- [4] A. Kristensen et al., Phys. Rev. B 62, 10950 (2000).
- [5] D. J. Reilly et al., Phys. Rev. B 63, 121 311 (2001).
- [6] S. Nuttinck *et al.*, Jpn. J. Appl. Phys. **39**, L655 (2000);
 K. Hashimoto *et al.*, Jpn. J. Appl. Phys. **40**, 3000 (2001).
- [7] D. Schmeltzer et al., Philos. Mag. B 77, 1189 (1998).
- [8] C.-K. Wang and K.-F. Berggren, Phys. Rev. B 57, 4552 (1998).
- [9] B. Spivak and F. Zhou, Phys. Rev. B 61, 16730 (2000).
- [10] H. Bruus, V.V. Cheianov, and K. Flensberg, Physica (Amsterdam) 10E, 97 (2001).
- [11] S. M. Cronenwett *et al.*, Phys. Rev. Lett. **88**, 226805 (2002).
- [12] D. Goldhaber-Gordon *et al.*, Nature (London) **391**, 156 (1998).
- [13] P.W. Anderson, Phys. Rev. 124, 41 (1961).
- [14] D. C. Langreth, Phys. Rev. 150, 516 (1966); see also T. K. Ng and P. A. Lee, Phys. Rev. Lett. 61, 1768 (1988).
- [15] J. R. Schrieffer and P. A. Wolff, Phys. Rev. 149, 491 (1966).
- [16] J. Kondo, Prog. Theor. Phys. 32, 37 (1964).
- [17] The parameters appearing in the Kondo Hamiltonian are not the bare parameters of the Anderson model (1), but renormalized parameters after the bandwidth has been reduced to U [F. D. M. Haldane, Phys. Rev. Lett. 40, 416 (1978)].
- [18] J. A. Appelbaum, Phys. Rev. **154**, 633 (1967). Appelbaum approximates the diverging integrals by $\log(|A| + k_b T)$. We use $\frac{1}{2}\log[A^2 + (k_b T)^2]$ instead.
- [19] P. Hohenberg and W. Kohn, Phys. Rev. 136, B864 (1964).
- [20] W. Kohn and L. J. Sham, Phys. Rev. 140, A1133 (1965). We use the local-density approximation for the exchange-correlation energy, parametrized for the twodimensional electron gas [B. Tanatar and D. M. Ceperley, Phys. Rev. B 39, 5005 (1989)].
- [21] J. Callaway and N. H. March, Solid State Phys. 38, 135 (1984).
- [22] The solution with broken spin symmetry coexists with an unpolarized solution [K. Hirose, N.S. Wingreen, and Y. Meir (to be published)]. See also A. M. Bychkov, I. I. Yakimenko, and K-F Berggren, Nanotechnology 11, 318 (2000).
- [23] D. Sprinzak et al., Phys. Rev. Lett. 88, 176805 (2002).
- [24] D. P. Pivin *et al.*, Phys. Rev. Lett. **82**, 4687 (1999); A. G. Huibers *et al.*, Phys. Rev. Lett. **83**, 5090 (1999).
- [25] J. A. Folk et al., Phys. Scr. T90, 26 (2001).