Kondo model for the “0.7 anomaly” in transport through a quantum point contact

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Experiments on quantum point contacts have highlighted an anomalous conductance plateau around 0.7(2e\textsuperscript{2}/h), with features suggestive of the Kondo effect. Here we present an Anderson model for transport through a point contact which we analyze 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 gate-voltage, temperature, magnetic-field, and bias-voltage dependence observed in the experiments. A strongly spin-polarized current is predicted for Zeeman splitting \(g^\star\mu_B B > k_B T_K, k_B T\).

The conductance through quantum point contacts (QPCs) is observed to be quantized in units of 2e\textsuperscript{2}/h. In addition to these integer conductance steps, an extra conductance plateau around 0.7(2e\textsuperscript{2}/h) has attracted considerable experimental effort and drawn attention to the effects of electron-electron interaction on the transport properties of low-dimensional quantum systems. Interaction effects in QPCs may enable novel applications such as solid-state spin filters, detection of a single charge and spin, and measurement and read-out of entangled spin states in quantum information devices.

A recent experiment 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, 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 \(g^\star\mu_B B > k_B T_K, k_B T\).

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 quasi-bound 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 quasi-bound state, resulting in a spin bound at the center of the QPC. We thus model the QPC and its leads by the Anderson Hamiltonian:

\[
H = \sum_{\sigma,k\in L,R} \varepsilon_{k\sigma} \hat{c}_{k\sigma}^\dagger \hat{c}_{k\sigma} + \sum_{\sigma} \varepsilon_{\sigma} \hat{d}_{\sigma}^\dagger \hat{d}_\sigma + U \hat{n}_\uparrow \hat{n}_\downarrow \\
+ \sum_{\sigma,k\in L,R} \left[ V_{k\sigma}^{(1)} (1 - \hat{n}_\sigma) \hat{c}_{k\sigma}^\dagger \hat{d}_\sigma + V_{k\sigma}^{(2)} \hat{n}_\sigma \hat{c}_{k\sigma}^\dagger \hat{d}_\sigma + H.c. \right]
\]

where \(\hat{c}_{k\sigma}^\dagger (\hat{c}_{k\sigma})\) creates (destroys) an electron with momentum \(k\) and spin \(\sigma\) in one of the two leads \(L\) and \(R\), \(\hat{d}_{\sigma}^\dagger (\hat{d}_\sigma)\) creates (destroys) a spin-\(\sigma\) electron on “the site”, i.e. the quasi-bound state at the center of the QPC, and \(\hat{n}_\sigma = \hat{d}_{\sigma}^\dagger \hat{d}_\sigma\). 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 step-like 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, \(\varepsilon_\uparrow = \varepsilon_\downarrow = \varepsilon_0\).

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 \(\varepsilon_F\) 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 $\approx 0.5$. Since $V_{k\alpha}^{(2)}$ may be significantly smaller than $V_{k\alpha}^{(1)}$, the contribution to the conductance from the $0 \leftrightarrow 2$ valence fluctuations may be small, until $\varepsilon_F \approx \varepsilon_0 + U$. However, the Kondo effect will 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 [19] for the Anderson model.

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 [10], so the Kondo limit of the Anderson Hamiltonian should be applicable. We therefore perform a Schrieffer-Wolff transformation [20] to obtain the Kondo Hamiltonian [21,22]

$$H = \sum_{\sigma,k \in L,R} \varepsilon_{k\alpha} c_{k\sigma}^\dagger c_{k\sigma} + \sum_{\sigma,j,k,k' \in L,R} (J_{kk'}^{(1)} - J_{kk'}^{(2)}) c_{k\sigma}^\dagger c_{k'\sigma}^\dagger c_{k'\sigma} c_{k\sigma} + 2 \sum_{\sigma,j,j' \in L,R} (J_{kk'}^{(1)} + J_{kk'}^{(2)}) (c_{k\sigma}^\dagger \sigma_{\sigma} \cdot \sigma_{\sigma}^\dagger c_{j\sigma}^\dagger S_j), \quad (2)$$

where $\varepsilon_{\sigma}^{(1)} = \varepsilon_{\sigma}$ and $\varepsilon_{\sigma}^{(2)} = \varepsilon_{\sigma} + U$. The Pauli spin matrices are indicated by $\sigma$, and the local spin due to the bound state is $\bar{S} = \sum_{\sigma} \bar{d}_{\sigma} \cdot \bar{d}_{\sigma}$. Following Appelbaum [23], we treat the above Kondo Hamiltonian perturbatively in the couplings $J_{kk'}^{(i)}$. The differential conductance to lowest order, $J^2$, is given by

$$G_2 = \frac{4\pi e^2}{h} \rho_{LR}(\varepsilon_F) \rho_{LR}(\varepsilon_F) \left\{ (J_{LR}^{(1)})^2 + (J_{LR}^{(2)})^2 \right\} \times \left[ 3 + 2 \langle M \rangle \left( \tanh \frac{\Delta + eV}{2k_B T} + \tanh \frac{\Delta - eV}{2k_B T} \right) \right], \quad (3)$$

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

$$J_{k'k}^{(i)} \equiv J_{k'k}^{(i)}(\varepsilon_F) = \frac{(-)^{i+1}V_k^2}{2(\varepsilon_F - \varepsilon_0)} f_{FD}(-\varepsilon_F/\delta), \quad (4)$$

where symmetric leads have been assumed, and the $V_i$ and $\delta$ are constants. The $J^{(i)}$ increase in a step of the Fermi-Dirac form $f_{FD}(x) = 1/[1 + \exp(x)]$. We define the combinations $J^{(i)}_{k'k} = J^{(i)}_{k'k} \pm J^{(i)}_{k'k}$ 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 $\rho_{LR}(\varepsilon) = \sum_{k \in L,R} \delta(\varepsilon - \varepsilon_k)$ is the single-spin electron density of states in the leads. We assume $\rho = \rho_L(\varepsilon) = \rho_R(\varepsilon)$.

As low temperatures the Kondo effect leads to a logarithmically diverging contribution $G_3$ (cf. [23]) to the differential conductance at order $J^3$, due to integrals running from the Fermi energy to either band edge. Because of the steplike increase of the $J^{(1)}$ band integral for $J^{(1)}$ runs down from $\varepsilon_F$ to the hybridization step at zero, but runs up from $\varepsilon_F$ 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 $G_3$.

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**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 $\varepsilon_F$ (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 different temperatures [11]. Center inset: Schematic of the band structure for our Anderson model. (b) Conductance in a magnetic field, for Zeeman splitting $\Delta = 0.07, 0.12, 0.4$ at $T = 0.06$ (solid curves from top to bottom). Inset: experimental conductance of QPC at different magnetic fields [12].

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The dependence of conductance on magnetic field is...
shown in Fig. 1(b). The Kondo logarithms in $G_3$ are suppressed and the term in $G_2$ that depends on $\langle M \rangle$ gives a negative contribution $\propto \tanh^2(\Delta/2k_B T)$, leading to the evolution of the 0.7 plateau towards and below 0.5. In agreement with experiment \cite{16}, the conductance is no longer monotonically increasing with Fermi energy $\varepsilon_F$: the energy denominator causes the $J^{(1)}$ contribution to $G_2$ to decrease, and this is no longer compensated by an increase of $G_3$. Due to shortcomings of perturbation theory the conductance at large magnetic field reduces to a value smaller than $0.5/(2e^2/h)$.

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 at weak magnetic fields ($\Delta > k_B T_K, k_B T$).

Lastly, we present evidence from spin-density-functional theory (SDFT) \cite{24} for the formation of a local moment (bound spin) at the center of a GaAs QPC, which supports our use of the Anderson model. SDFT is applied within the local-density approximation \cite{24,26}. The external potential consists of a clean quantum wire with a parabolic confining potential of $V_0 = (1/2)\hbar^2\omega_y^2 y^2$ and a QPC potential

$$V_{\text{QPC}}(x, y) = V(x)/2 + m^* |V(x)/\hbar|^2 y^2/2,$$  \hspace{1cm} (6)

where $V(x) = V_0/\cosh^2(\alpha x)$, with $\alpha = \omega_x/\sqrt{m^*/2\hbar V_0}$. 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 \cite{24} 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 $\hbar\omega_y = 2.0\text{meV}$. The parameters for the QPC potential are taken to be $V_0 = 3.0\text{meV}$ and $\hbar\omega_x = 1.5\text{meV}$.

Fig. 3(a) shows the spin-dependent, self-consistent QPC barriers at $T=0.1\text{K}$ obtained from SDFT \cite{27}. Specifically, we plot the energy of the bottom of the lowest 1D subband $\varepsilon_\sigma(x)$, relative to the value $\varepsilon_0$ far into the wire, for both spin-up and spin-down. The local density of states $\nu(\varepsilon)$ at the center of the QPC is shown for both spin-up and spin-down in the right inset. Fig. 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 quasi-bound state centered at the QPC: there is a resonance in the local density of states $\nu(\varepsilon)$ for spin-up, with a net of one spin bound in the vicinity of the QPC. The transmission coefficient $T(\varepsilon)$ for electrons in the lowest subband is shown in the left inset to Fig. 3(a). Transmission for spin-up is approximately 1 over a broad range of energies above the spin-up resonance. This implies an onset of strong hybridization at energies above the quasi-bound state.

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 ↔ 1 valence transitions account for the background conductance, while 1 ↔ 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 $k_B T$ and $k_B T_K$. 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 $G \approx e^2/h$, i.e. in the region of maximal sensitivity to its environment. When the gate voltage controlling the other point contact 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 pinch-off 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 [22], and may complicate attempts to measure the spin of dot electrons. [30].

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

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Fig.3: Results of spin-density-functional theory. (a) Self-consistent “barrier”, i.e. energy of the bottom of the lowest 1D subband at temperature $T = 0.1K$ as a function of position $x$ in the direction of current flow through the QPC. The electrochemical potential $\mu$ 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 spin-averaged density. Inset: contour plot of the QPC potential $V_{QPC}(x,y)$.

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)].

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where $\varepsilon_{xc}[\rho(r)]$ is the parameterized form by Tanatar and Ceperley for the two-dimensional electron gas [B. Tanatar and D. M. Ceperley, Phys. Rev. B\textbf{39}, 5005 (1989)].

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