Singular conductance of a spin 1 quantum dot

A. Posazhennikova

1 Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, 76128 Karlsruhe, Germany

2 Center for Materials Theory, Rutgers University, Piscataway, NJ 08855, U.S.A.

We interpret the recent observation of a zero-bias anomaly in spin-1 quantum dots in terms of an underscreened Kondo effect. Although a spin-1 quantum dots are expected to undergo a two-stage quenching effect, in practice the log normal distribution of Kondo temperatures leads to a broad temperature region dominated by underscreened Kondo physics. General arguments, based on the asymptotic decoupling between the partially screened moment and the leads, predict a singular temperature and voltage dependence of the conductance G and differential conductance dG/dV, resulting in dg/dT ∼ 1/T and dG/dV ∼ 1/V. Using a Schwinger boson approach, we show how these qualitative expectations are borne out in a detailed many body calculation.

PACS numbers: 72.15.Qm, 73.23.-b, 73.63.Kv, 75.20.Hr

Single-electron transistors (SETs) offer the intriguing opportunity to probe and explore classes of strongly correlated electron behavior associated with the Kondo effect that are difficult to access in bulk materials. The possibility of observing a breakdown in Landau Fermi liquid behavior that accompanies the Kondo effect has been a subject of particular recent interest. In this paper, we propose that singular deviations from Landau Fermi liquid behavior that accompanies the two-channel Kondo effect in quantum dots has been a subject of particular recent interest. In this paper, we propose an interpretation of this unexpected behavior in terms of an underscreened Kondo effect. Our key observation is that the antiferromagnetic Kondo coupling constants will drive a log-normal distribution in Kondo temperatures of each channel, with the potential to generate exponentially large separations in the relative magnitude of the Kondo temperatures of each channel.

If we assume that ln(T_{K1}/T_{K2}) = \frac{1}{J_{x\rho}} - \frac{1}{J_{y\rho}} >> 1, then over the exponentially broad temperature range given by log(T_{K1}) >> log T >> log(T_{K2}), the underlying physics is that of a one channel spin-1 Kondo model, in which the spin is partially screened to a spin 1/2.

From this perspective, triplet dots with a large zero bias anomaly are those where the Kondo coupling constants of the two channels are severely mis-matched, giving rise to decades of behavior dominated by the underscreened Kondo effect in a single channel. Previous work, both analytic and numerical, has focussed on the equilibrium behavior of triplet quantum dots with Kondo temperatures of comparable magnitude. We now examine the singular consequences of a wide separation...
between these two scales in both finite temperature and finite voltage properties.

In the underscreened spin-1 Kondo effect, the residual spin-1/2 moment is ferromagnetically coupled to leads, with a coupling that scales logarithmically slowly to zero \[ H = H_0 + \sum_{k,l} \epsilon_{kl} c_k^\dagger \sigma \cdot S, \]
where \[ H_0 = \frac{1}{\ln(\frac{T}{K})} + O \left( \frac{1}{\ln(\frac{T}{K})} \right) \]
where \[ \Lambda = \text{max}(T, \mu_B B) \] is the characteristic cut-off energy scale, provided in equilibrium, by the temperature or magnetic field. At low energies and temperatures, the spin is partially screened from spin \( S \) to spin \( S - (1/2) \). The residual moment is ferromagnetically coupled to the conduction sea, with a residual coupling that slowly flows to weak coupling according to

These singular features of the underscreened Kondo effect are expected to manifest themselves in the properties of the triplet quantum dot. For example, we expect the low-field conductance to follow the simple relation

\[
G(B) = \frac{2e^2}{h} \sin^2 \delta(B) \sim \frac{2e^2}{h} \left( 1 - \frac{\pi^2}{16 \ln^2 \left( \frac{T_K}{B} \right)} \right),
\]
for \( B << T_K \). This relationship was previously obtained by other means from the \( T_K \) to \( 0 \) of the two-channel model. Notice that the field derivative of the conductance diverges as \( \frac{dG}{dB} \propto 1/ \left( B \ln^3(T_K/B) \right) \) at low fields. The prediction of the finite temperature, and finite voltage conductance cannot be made exactly, however we expect the above form to hold, for the differential conductance at finite temperature or voltage, with an appropriate replacement of cut-off, namely

\[
G(V,T) \sim \frac{e^2}{h} \left( 1 - \frac{\pi^2}{16 \ln^2 \left( \frac{T}{\max(T,V)} \right)} \right)
\]

and \( dG/dT \sim 1/\max(T,V) \).

To model this behavior in more detail it is useful to consider a simplified model of the quantum dot in which the Hund’s coupling is taken to be infinite. In this limit, the states of the quantum dot can be described using a Schwinger boson representation

\[
|d^1, \sigma\rangle = b_{\sigma}^\dagger \chi^\dagger |0\rangle, \quad |d^2, M\rangle = b_{\pi}^\dagger b_{M-\pi}^\dagger |0\rangle,
\]
Written in this representation the model becomes

\[
H = H_0 + t \sum_{\sigma} \left[ \psi_{\sigma}^\dagger \chi^\dagger b_\sigma + b_\sigma \chi \psi_\sigma + E_d \xi_\sigma \chi \right].
\]
subject to the constraint \( n_\sigma + \chi^\dagger \chi = 2 \).

To develop a controlled many body treatment of this Hamiltonian, we use a large-\( N \) expansion, extending the number of spin components \( \sigma \) from two to \( N \). To preserve a finite scattering phase shift as \( N \rightarrow \infty \), we introduce \( K = kN \) bosonic “replicas”, where \( k \) is fixed. With this device we obtain a (dynamical) mean field theory with scattering phase shift \( \delta = \pi k \) and the qualitatively correct logarithmic energy dependencies. The Hamiltonian used in the large \( N \) expansion is then

\[
H = H_0 + \frac{i}{\sqrt{N}} \sum_{\sigma,\mu} \left[ \psi_{\sigma}^\dagger \chi_\mu^\dagger b_\sigma + b_\sigma \chi_{\mu} \psi_\sigma + E_d \sum_{\mu=1}^{kN} \chi_\mu \chi_{\mu}\right]
\]

In the large \( N \) limit, there are two self-consistent non-crossing approximations to the Dyson equations for the self-energies of the conduction electrons and \( \chi \) fermions (Fig. 1). Here we sketch the main elements of the derivation. As in the corresponding equilibrium calculation, the boson behaves as a sharp excitation in the large \( N \).
limit, with an average occupancy \(\langle n_{b\sigma\mu}\rangle = n_b/N\). From the Dyson equations we obtain sets of self-consistent integral equations for both the retarded and Keldysh self-consistently determines the fermion distribution functions. We can summarize the results of our calculation, the number of bound bosons in the Kondo singlet never exceeds \(N/2\) and the region \(K \geq N/2\) does not

\[
\begin{align*}
\Sigma_R^c(\omega) &= -\tilde{t}^2 n_b G_A(\lambda - \omega) - \tilde{t}^2 \int \frac{d\omega'}{\pi} f_c(\omega') \frac{1}{\omega' + \omega - \lambda + i\delta} \text{Im} G_R(\omega'), \\
\Sigma_R^r(\omega) &= -\tilde{t}^2 k n_b J_A(\lambda - \omega) - \tilde{t}^2 k \int \frac{d\omega'}{\pi} f_X(\omega') \frac{1}{\omega' + \omega - \lambda + i\delta} \text{Im} J_R(\omega').
\end{align*}
\] (10)

Here \(J_R(\omega) = [\omega - E_d - \Sigma_R^c(\omega)]^{-1}\) and \(G_R^c(\omega) = \left[(\pi \rho)^{-1} - \Sigma_R^c(\omega)\right]^{-1}\) are the retarded propagators for the \(\chi\) fermions and conduction electrons.

![FIG. 1: The non-crossing approximation for the self-energies of conduction electrons and \(\chi\) fermions. The solid line denotes the Larkin Ovchinnikov matrix propagator for the conduction electrons. The dashed line denotes the corresponding Green’s function of the auxiliary \(\chi\) fermions and the wavy line is the bosonic propagator. Thin lines denote the bare propagator and full lines the dressed propagator. Each vertex corresponds to the factor \(\frac{1}{i\pi}\).

The ratio of the Keldysh to the retarded self-energies self-consistently determines the fermion distribution functions. We can summarize the results of our calculation of the Keldysh self-energies by providing the distribution functions that they generate. The distribution function of the conduction electrons is the average

\[
f_c = \frac{1}{2} \left[f_L(\omega) + f_R(\omega)\right],
\] (11)

where \(f_{L,R}(\omega) = 1/(e^{\beta(\omega + eV)/2} + 1)\) is the equilibrium distribution function in the left/right-hand lead. The distribution function of the auxiliary fermion is

\[
f_X(\omega) = \frac{n_b[1 - f_c(\omega)]}{n_b + f_c(\omega)}.
\] (12)

where \(n_b = 1/(e^{\beta \lambda} + 1)\) determines \(\lambda\). This relationship can be simply understood as the result of detailed balance between rate of the decay processes \(c \to b + \chi\) and \(b + \chi \to c\), and it reverts to the equilibrium Fermi Dirac distribution in the limit \(V \to 0\). From these results, we compute the temperature and voltage dependent current, given by

\[
I(V,T) = \frac{\pi^2 V^2}{h} \int d\omega \frac{\left[f_L(\omega) - f_R(\omega)\right]}{eV} \text{Im} t_{LR}(\omega)
\] (13)

where \(t_{LR}(\omega) = \Sigma_R^c(\omega) / [1 - i\pi \rho \Sigma_R^c(\omega)]\) is the scattering t-matrix.

We have solved these equations numerically, and the key results are shown in Figs 2-4. Fig. 2. shows the voltage dependent current, given by

\[
I(V,T) = N \frac{\pi^2 V^2}{\hbar} \int d\omega \frac{\left[f_L(\omega) - f_R(\omega)\right]}{eV} \text{Im} t_{LR}(\omega)
\]

FIG. 2: Imaginary part of dot T-matrix for a variety of voltages for the case \(k = 0.4\). As the voltage is increased, the singular central peak splits into two components.
describe an underscreened Kondo model. Consequently, we are limited to static phase shifts $\delta = \pi(K/N) < \pi/2$, so the strictly particle-hole symmetric case $\delta = \pi/2$ is outside the limits of our approach. Nevertheless, our numerical results do capture the expected singularities. Fig. 3. shows the singular form of the temperature dependence of the differential conductance, with singular $1/T$ divergence in $dg/dT$. Finally, Fig. 4. shows the voltage dependence of the conductance, which has a similar logarithmic singularity at low voltage.

In summary, we have proposed that the monotonically increasing conductance observed as the temperature is lowered in triplet quantum dots is associated with an underscreened Kondo effect. The singular energy and temperature dependence associated with the Kondo resonance is predicted to give rise to a $1/T$ divergence in the temperature dependence of the differential conductance, and a $1/V$ divergence in the second derivative of the voltage dependent current $d^2I/dV^2$. These ideas have been developed qualitatively and illustrated within an integral equation treatment of the underscreened Kondo model. Experimental observation of these singular features would constitute a first realization of the underscreened Kondo effect.

The authors wish to thank H. Kroha, G. Zarand and M. Eschrig for discussions related to this work. This research was partly supported by the Alexander Von Humboldt foundation (AP) and DOE grant DE-FG02-00ER45790 (PC).

[1] Leo Kouwenhoven and Leonid Glazman, Physics World 14, 33 (2001).
[2] L. I. Glazman and M. E. Raikh, JETP Lett. 47, 452 (1988).
[3] T. K. Ng and P. A. Lee, Phys. Rev. Lett. 61, 1768 (1988).
[4] D. Goldhaber-Gordon, Hadas Shtrikman, D. Mahalu, David Abusch-Magder, U. Meirav and M. A. Kastner, Nature 391, 156 (1998)
[5] S.M. Cronenwett et al., Science, 281, 540 (1998).
[6] Yuval Oreg, David Goldhaber-Gordon, Phys. Rev. Lett. 90, 136602 (2003).
[7] M.G. Vavilov, L.I. Glazman, cond-mat/0404366, (2004).
[8] J. Schmid, J. Weis, K. Eberl, and K. v. Klitzing, Phys. Rev. Lett. 84, 5824 (2000).
[9] S. Sasaki, S. De Franceschi, J. M. Elzerman, W. G. van der Wiel, M. Eto, S. Tarucha and L. P. Kouwenhoven, Nature 405, 764 (2000).
[10] A. Kogan, G. Granger, M. A. Kastner, D. Goldhaber-Gordon, H. Shtrikman, Phys. Rev. B 67, 113309 (2003).
[11] M. Pustilnik and L. I. Glazman, Phys. Rev. Lett. 87, 216601 (2001).
[12] W. Hofstetter, G. Zarand, Phys. Rev. B 69, 235301 (2004).
[13] O. O. Bernal, D. E. MacLaughlin, H. G. Lukefahr, B. Andraka, Phys. Rev. Lett. 75, 2023 (1995); R. N. Bhatt and D. S. Fisher, Phys. Rev. Lett. 68, 3072, 1992; V. Dobrosavljevic, T. R. Kirkpatrick and G. Kotliar, Phys. Rev. Lett. 69, 1113 (1992).
[14] W. Hofstetter & Herbert Schoeller, Phys. Rev. Lett. 88, 016803 (2002)
[15] P. Nozières, Journal de Physique C 37, C1-271, 1976 ; P. Nozières and A. Blandin, Journal de Physique 41, 193, 1980.
[16] P. Coleman and C. Pepin, Phys. Rev. B 68, 220405(R) (2003).
[17] Pankaj Mehta, L. Borda, G.Zarand, N. Andrei, P. Coleman, cond-mat/0404122 (2004).
[18] I. Paul and P. Coleman, cond-mat/0404001 (2004).
[19] Y. Meir and N. S. Wingreen, Phys. Rev. Lett. 68, 2512 (1992).