Anomalous Kondo Spin Splitting in Quantum Dots

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The Zeeman splitting of localized electrons in a quantum dot in the Kondo regime is studied using a new slave-boson formulation. Our results show that the Kondo peak splitting depends on the gate potential applied to the quantum dot and on the topology of the system. A common fact of any geometry is that the differential susceptibility shows a strong non linear behavior. It was shown that there exist a critical field above which the Kondo resonance is splitted out. This critical field rapidly diminishes when the gate potential is lowered, as a consequence of the reduction of the Kondo temperature and a subsequent strong enhancement in the differential susceptibility occurring at low fields. The critical field is also strong dependent on the topology of the circuit. Above this critical field the Zeeman splitting depends linearly upon the magnetic field and does not extrapolate to zero at zero field. The magnitude of the Y-intercept coordinate depends on the gate potential but the slope of this function is not renormalized being independent of the value of the gate potential.

Our results are in agreement with very recent experiments.

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The observation of Kondo effect in quantum dots has already a large history.\[\text{(1, 2)}\] The effect appears when a net spin becomes localized at a quantum dot (QD) coupled with metallic leads.\[\text{(3, 4)}\] Local spin fluctuations (LSF) in the vicinity of the QD allows the spin of the electrons in the leads to screen the localized spin, as a magnetic impurity is screened in a host metal. A sharp resonance in the local density of states (LDOS) is developed at the Fermi level of the system. When the QD is connected as a bridge between two metallic leads, the embedded geometry (EG), the resonance provides a channel of conduction and the conductance reaches the value \(G = 2G_0\), being \(G_0 = \frac{e^2}{2h}\) the quantum of conductance. When the QD is side connected (SCG), two channels of conduction interfere destructively (one direct and other across the QD, from lead to lead) and the conductance is zero for the value of the gate potential, for which the interference is complete. The existence and characteristics of the Kondo resonance can be studied through conductance \(G\) of the system.

To better understand the Kondo effect it is important to study its behavior when an external magnetic field is applied. It is expected the LSF to be quenched and the Kondo regime to disappear for large enough fields. For intermediate values, the Kondo resonance is splitted and its effect can be observed in the differential conductance of the system.\[\text{(2)}\] In recent experiments\[\text{(5, 6)}\] it was possible to obtain very precise value of \(\Delta\), the Zeeman splitting, (ZS) for localized electrons in a QD in the Kondo regime (KR). However, these experiments are controversial. In one of them,\[\text{(2)}\] above a critical value of the magnetic field, it was found that \(\Delta \sim \Delta_B = 2g\mu_BB\), where \(g, \mu_B\) and \(B\) is the gyromagnetic factor, the Bohr magneton and the magnetic field respectively. In others,\[\text{(3, 4, 5)}\] below a critical value, the effect of the magnetic field was not observed and above it the splitting was larger than \(\Delta_B\) and does not extrapolate to zero at zero field.

The splitting was initially theoretically predicted\[\text{(6)}\] to be \(\pm g\mu_BB\), in line with\[\text{(2)}\]. However, more recent calculations\[\text{(5)}\] shows that the splitting would be observable only above \(B_c\), when the magnetic Zeeman energy \(\Delta_B\) becomes competitive with the Kondo temperature \(T_K\). Moore and Wen\[\text{(7)}\] established the relationship between the field induced spin splitting in the spectral function of the system in equilibrium and the splitting appearing in the differential conductance when the system is slightly out of equilibrium. They predict also that the spin screening characteristic of the KR should reduce the magnetic field splitting, \(i.e, \Delta < \Delta_B\). Unfortunately these theories were not capable of explaining the phenomenology seen in the latest experiments\[\text{(5, 6)}\].

In this letter we developed a theoretical study that correctly explains these last experimental results. We use different approaches to study the problem. We propose a new slave-boson formalism(SB) that considers two independent boson fields, each one associated to up and down spin. We solve the problem using as well the embedded cluster method (ECM), which is a powerful tool to study strong correlated systems\[\text{(11)}\], and we compare the results of these two approaches. We study the system for the two geometries mentioned above (side connected and embedded). The value of the splitting results to be dependent on the geometry of the circuit and has a strong dependence on the gate potential applied to the QD and...
the coupling between the leads and the QD. We also obtain the solution in the Hubbard I (HI) approximation that adequately describes the situation for \( T > T_k \).

The system is described by the Anderson impurity Hamiltonian including the effect of an external magnetic field. We identify three contributions to the total Hamiltonian: the leads \( (H_L) \), the QD term \( (H_C) \) and the connections among the leads and the dot \( (H_T) \). \( H_L \) is the Hamiltonian of two semi-infinite chains for the EG configuration or of a one dimensional infinite chain for the SCG case. The Hamiltonian \( H_C \) is given by,

\[
\hat{H}_C = \sum_\sigma \epsilon_\sigma n_{0,\sigma} + U n_{0,\uparrow} n_{0,\downarrow}
\]

(1)

where the subindex 0 denotes the QD site, \( \epsilon_\pm = V_g \pm B \) is the spin dependent QD energy level, \( V_g \) is the gate potential at the QD site and \( U \) the Coulomb repulsion that, for simplicity, is supposed to be infinite. We have adopted \( |g\mu_B| = 1 \). Finally,

\[
\hat{H}_T = \sum_{i,\sigma} \left[ V a_{i,\sigma}^\dagger c_0 \beta_{\sigma} \right] + c.c.
\]

(2)

where \( i = -1 \) and 1 for EG or \( i = 1 \) for the SCG. In the first case \(-1 \) and 1 denotes the first site of the left and right semi-infinite one dimensional leads. In the second case 1 is the site of an infinite one dimensional lead to which the QD is connected and \( V \) is the hopping probability (see Fig. 1). All the energies are expressed in units of the hopping among the leads sites \( t \), \( D \) denotes the bandwidth of the leads and the Fermi energy is \( E_f = 0 \). In the new slave-boson formulation we define a boson field associate to each electron spin. The fermion operators \( a_{i,\sigma}^\dagger \) is written as the product, \( a_{i,\sigma}^\dagger = c_{i,\sigma}^\dagger b_{i,\sigma}^\dagger \), where \( c \) and \( b \) denote the quasi-fermion and boson operators. Following a similar formulation to the standard one \[12\], \( H_T \) is transformed into

\[
\hat{H}_T = \sum_{i,\sigma} \left[ V a_{i,\sigma}^\dagger c_0 \beta_{\sigma} \right] + c.c.
\]

(3)

In order to avoid double occupancy at the QD, constraint conditions have to be imposed. They are written,

\[
2n_{0,\sigma} + b_{i,\sigma}^\dagger b_{i,-\sigma} + b_{i,-\sigma}^\dagger b_{i,\sigma} = 1.
\]

(4)

When both spins are equivalent, the above equations merge into the constraint of the standard slave-boson formalism. The Hamiltonian is treated in the mean-field approximation for the boson fields (MFSB), substituting in equations (3) and (4) the operator \( b_\sigma \) by its mean-value \( z_\sigma = \langle b_\sigma \rangle \). The mean-field versions of equations (4) are incorporated into the Hamiltonian using the Lagrange multipliers \( \gamma_\sigma \). Minimizing the total energy with respect to these multipliers we obtain two new equations,

\[
KV < a_{1,\sigma}^\dagger c_0 > + z_\sigma^2 (\gamma_\sigma + \gamma_{-\sigma}) + \gamma_\sigma - \gamma_{-\sigma} = 0
\]

(5)

where \( K = 1 \) for the SCG and \( K = 2 \) for the EG. We solve equations (5) self-consistently and obtain the Green function at the QD and the transmission \( T(E) \) across it ( \( G = T(E_f) \)).

We have chosen the parameters to obtain a similar Kondo resonance for the SCG and the EG configurations. They are \( V = 0.35 \) for the EG and \( V = 0.65 \) for the SCG. Increasing \( V_g \) the system goes from Kondo to mixed valence regime.

Fig. 2 (upper panels) shows the transmission at zero field obtained using the approximations MFSB and ECM. The effect of the Kondo resonance is clear: \( G = 2 \) or \( G = 0 \) for the EG or the SCG configurations respectively, and a resonance or anti-resonance width roughly similar for both geometries and both methods of calculations. When the magnetic field is increased the Kondo peak is splitted and eventually the system goes out of resonance. In the medium panels of Fig. 2 we show the transmission for \( B = 0.18 \). The value of the magnetic field splitting obtained by the two methods are very similar, and for the ECM the results are almost independent of the cluster size exactly diagonalized.

To study how this splitting develops we write down the expression for the Green function at the QD. For the MFSB solution we have,

\[
G_{0,\sigma}(E) = \frac{1}{E - \epsilon_\sigma - 2\gamma_\sigma + K(V z_\sigma)^2 g_{\sigma L}(E)}
\]

(6)

Here \( g_{\sigma L}(E) \) is the undressed Green function of the lead. From equation (6) we can obtain \( E_\sigma \), the values of the renormalized energies of the QD level. They are,

\[
E_\sigma = \frac{\epsilon_\sigma + 2\gamma_\sigma}{1 - ((K - 1)(V z_\sigma/t))^2}.
\]

(7)
The term $\Gamma_\sigma = \frac{2\gamma_\sigma}{1-(K-1)(V z_\sigma)^2}$ can be interpreted as the spin dependent renormalization of the resonance level by the interaction. Depending on the geometry ($K = 1$ or 2) there is also a multiplicative correction in the term $\epsilon_\sigma$. The ZS is given by the difference $\Delta = E_\downarrow - E_\uparrow$.

$$\Delta = \frac{V_g + B + 2\gamma_\downarrow}{1-(K-1)(V z_\downarrow)^2} - \frac{V_g - B + 2\gamma_\uparrow}{1-(K-1)(V z_\uparrow)^2}$$  \hspace{1cm} (8)

In Fig. 3 and 4 (lower panel) we show the parameters of the problem as a function of the magnetic field. For both configurations $z_\uparrow \rightarrow 1, z_\downarrow \rightarrow 0$ when $B \rightarrow \infty$. $\Delta$ and $\Delta_\Gamma = \Gamma_\downarrow - \Gamma_\uparrow$ show a rapid increase at low fields, more evident for the SCG case. $\Delta_\Gamma$ results to be almost constant for a large range of values of the magnetic field. As a consequence, $\Delta(B)$ tends asymptotically to a linear function. The slope of this linear function is qualitatively the same as for the non-interacting regime (for the EG configuration there is a small correction proportional to $V^2$ with respect to the non-interacting case). For low fields, $\Delta$ rises due to the Zeeman effect but also because the local level at the QD suffers a spin dependent renormalization as the magnetic field progressively quenches the LSF, giving an additional contribution to the splitting. The differential magnetic susceptibility (DMS) is strongly enhanced for low magnetic fields, (see the curve $n_0, \uparrow - n_0, \downarrow = \Delta_\sigma$ in figures 3,4). For larger fields, when the spin fluctuations are quasi totally suppressed, $\Delta$ recovers its linear function appearance, but shifted up with respect to the origin, due to the Coulomb interaction acting on each spin level. Lowering $V_g$, the Y-intercept coordinate of this linear function is increased, although the slope does not change. For a fixed value of the field $B$, $\Delta$ results to depend linearly on $V_g$ with a slope $\alpha$ almost independent of $B$ (see the inset of figures 3 and 4). This implies that, as known, $\Delta$ increases logarithmically by lowering the Kondo temperature since $V_g \sim (V^2/D)\log(D/T_k)$. As $\Delta > \Delta_B$, the slope $\alpha$ is larger than the value predicted in [8], and in agreement with recent experiments [9, 10]. Increasing $V_g$, we enter into the mixed valence regime and $\Delta$ recovers a nearly linear evolution that almost extrapolates to the origin. In this regime $\Delta_\Gamma$ is not constant anymore but increases monotonically with the field. As a consequence, the slope of the linear relationship between $\Delta$ and $B$ is renormalized for both geometries with respect to the non-interacting case. In spite of this, it is important to realize that $\Delta$ is always lower than the value it acquires in the Kondo regime.

To determine when the ZS can be experimentally detected the relevant quantity to be study is $W$, the semi-sum of the resonance width of each Kondo peak. It can be expressed as,

$$W = K \left[ \frac{(V z_\downarrow)^2}{1-(K-1)(V z_\downarrow)^2} + \frac{(V z_\uparrow)^2}{1-(K-1)(V z_\uparrow)^2} \right]$$  \hspace{1cm} (9)

The ZS is not detectable if $\Delta < W$. The value of the critical magnetic field $B_c$ satisfies the equation $\Delta(B_c) = W(B_c)$. In figure 3 and 4 we plot $W(B)$ for $V_g = -0.5$ and $V_g = -0.4$, respectively. The values of $W$ obtained from (9) at $B = 0$ are the same to those obtained with the usual formula $T_k = Dexp(-x V_g/2K V^2)$ [12] where $x$ is $\pi$ for EG or $2\pi$ for SCG. The $B_c$ obtained for each configuration corresponds to a $\Delta(B_c) << T_k$ in line with the
experimental observation. Note that \( B_c \) is appreciably smaller for the SCG than for the EG topology because in this case \( \Delta \) has a negative contribution comming from smaller for the SCG than for the EG topology because more rapid increasing with \( B \). \( \Delta \) shows \( \Delta(B) \) for two magnetic fields. Lower panel: evolution of the parameters with \( B \), for \( V_g = -0.5 \). The inset shows \( \Delta(V_g) \) for two magnetic fields.

We have also solved the problem in the Hubbard I approximation. It describes the situation for each geometry. (lower pannels) it is shown how the splitting develops for each geometry.

We can determine the position of the resonances as a function of the external field \( B \). \( \Delta \) results to be:

\[
\Delta = \frac{V_g + B}{1 - (K - 1)V^2(1 - n_f)} - \frac{V_g - B}{1 - (K - 1)V^2(1 - n_i)}
\]

The function \( \Delta(B) \) is plotted in figures 3 and 4. The remarkable fact is that for the SCG configuration the slope is equal to that of the low temperature solutions obtained with MFSB, while for the EG there is a small renormalization of it. This shows that the essential difference between the low and high temperature regime as far as the ZS is concerned is the existence of a non-zero Y-intercept coordinate at low temperatures as has been seen in the experiment. In spite of the similar behavior of the slope of the function \( \Delta(B) \), the magnetization in this high temperature regime is very different. The DMS at zero field is much less at high temperature than at low temperature.

Summarizing, we have studied the magnetic response of a QD connected with two different geometries SCG and EG. To do so we developed a slave-boson formalism that takes into account a different boson field for each spin. In the Kondo regime there is a critical magnetic field \( B_c \) above which the Kondo resonance can be seen splitted. \( B_c \) depends upon the topology of the system, being larger for the EG than for the SCG configuration. The Zeeman energy associated to this field is lower that the Kondo temperature. For \( B < B_c \), \( \Delta \) suffers a non-linear and rapid growth with the magnetic field that occurs due to the spin dependent local energy Coulomb renormalization and the quenching of the LSF induced by the magnetic field. When the spin fluctuations are completely quenched, \( B > B_c \), the spin splitting is proportional to the magnetic field with a slope independent on temperature and gate potential. The Y-interception coordinate is non zero and increases when the gate potential is reduced. At a fixed magnetic field, \( \Delta(V_g) \) results to be a linear function with a \( B \) independent slope. The value of \( \Delta \) is always greater than \( \Delta_B \) for \( T < T_k \) due to the spins correlations implied in the Kondo effect. Our results are in good agreement with recent experimental results.

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**FIG. 4:** Results for the SCG. Upper panel: The function \( \Delta(B) \) for three different values of \( V_g \). The semi-sum of the resonance widths \( W \), for \( V_g = -0.5 \), is shown with thick trace line. The equation \( W(B) = \Delta(B) \) defines \( B_c \). The point line shows \( \Delta \) using the Hubbard I approximation. Lower panel: evolution of the parameters with \( B \), for \( V_g = -0.5 \). The inset shows \( \Delta(V_g) \) for two magnetic fields.

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