Possibility of Two-channel Spin $\frac{1}{2}$ Kondo Conductance in a Quantum Dot

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Abstract. – By combining exact diagonalization with scaling method, we show that it is possible to realize two channel spin $\frac{1}{2}$ Kondo (2CK) conductance in a quantum dot at Coulomb Blockade, with an odd number of electrons and with contacts in a pillar configuration, as an applied orthogonal magnetic field $B$ is tuned at an appropriate level crossing.

A Quantum Dot (QD) weakly coupled to the contacts and tuned in a valley between two conduction peaks (Coulomb Blockade (CB)), is insulating if its charging energy is larger than the thermal energy $k_B T$. However, when the number of electrons at the dot, $N$, is odd, below a characteristic temperature scale $T_K$, a strongly correlated state between the dot and the contacts sets in, and the typical Kondo resonance in the conduction electron spectral density builds up at the chemical potential of the contacts $\mu$. The striking result is that the linear conductance increases in the CB valley, when the temperature $T$ is lowered, up to the unitarity limit $2e^2/h$ for $T = 0$. If $N$ is even, the ground state (GS) of the QD is usually a spin singlet and the ordinary Kondo effect cannot occur. Nevertheless, it has been shown that level crossing between states at different $S$ induced by a magnetic field $B$ orthogonal to the dot can restore the degeneracy required for the Kondo effect to take place. The occurrence of Kondo physics in quantum dots was predicted long ago in analogy to magnetic impurities in diluted metal alloys at very low temperatures. A dot at CB acts as a single magnetic impurity, but under controlled experimental conditions.

A realistic description of the Kondo effect in alloys has to take into account that the impurity states carry also orbital angular momentum together with spin momentum. Hence, electrons with different orbital momentum can access the impurity and both multi-orbital 1-channel Kondo Effect (1CK) and many-channel Kondo effect (MCK) can take place. Total angular momentum is conserved in the scattering, as it is appropriate for an atomic impurity in an isotropic metal.

Similarly to the ordinary 1CK, MCK shows a logarithmic low-temperature raise in the resistivity before the perturbative expansion breaks down ($T \sim T_K$). However, if the number...
Fig. 1 – (a): Sketch of the dot. (b) Sketch of the conductance as a function of the temperature $T$ and the gate voltage $V_g$. At $2CK$ non Fermi liquid point, the conductance shows a $\sqrt{T}$ dependence.

of channels $k > 2S$ (overscreening), the physics of the two systems at $T \ll T_K$ is dramatically different. The overscreened impurity interacts again antiferromagnetically with the other conduction electrons. Accordingly, the strongly coupled antiferromagnetic (AF) fixed point becomes unstable at $T = 0$ and moves to intermediate coupling. The Fermi-liquid phase breaks down and leading corrections to the resistivity $\rho(T)$ are characterized by a non-Fermi liquid square-root temperature dependence $[9]$. The prototype of this situation is an $S = \frac{1}{2}$ impurity interacting with two channels of conduction electrons.

Possibly, $2CK$ zero-bias conductance anomaly has been detected in transport measurements in $Ti-$ and $Cu-$ nanoconstrictions with controlled doping, with $T_K$ between 0.5 K and 4.6 K $[10]$. Also, interstitial atoms in glassy metals could be described as tunneling two-level systems (TLS) and they could give rise to $2CK$ by scattering with conduction electrons $[11]$. However, a careful estimate of the Kondo temperature in these materials is still a widely debated question and appears to give a value below $10^{-4}$ K $[12]$.

In this letter we propose to search for $2CK$ spin $\frac{1}{2}$ in a quantum dot (QD) biased at Coulomb blockade with odd $N$ and total spin $S = 1/2$. We discuss the geometry, the working conditions, and the most appropriate energy level structure to achieve $2CK$ within the limits of present technology.

We consider a QD in a pillar configuration with cylindrical symmetry about the $z$-axis (see Fig.1 a ). We label dot states with total energy $NE_i$ ( $i = 0$ for the GS) and total angular momentum $M$ along the $z$ axis. By means of single-electron tunneling with the contacts, the dot can exchange orbital momentum $m$ and/or spin $\sigma$ with conduction electrons. We describe a particular scenario derived from results of an exact diagonalization of electrons in a two-dimensional parabolic confining potential with Coulomb interaction energy scale $U$ $[13]$. The addition energies of the dot can be shifted with respect to $\mu$ by tuning a gate voltage $V_g$. The field $B$ orthogonal to the dot can induce strong orbital effects, which may eventually give raise to crossings between states with different $M$ and $S$. The dot is tuned at CB with $N = 5$ at $B^*$ where two $S = \frac{1}{2}$ levels with $M = 4$ and $M = 6$ cross (Fig.2 ).
possibility of two-channel spin $\frac{1}{2}$ Kondo conductance in a quantum dot.

Within the subspace $\Xi$ spanned by the states $|N, M, S_z\rangle = |5, 4, \pm \frac{1}{2}\rangle$ and $|5, 6, \pm \frac{1}{2}\rangle$, the QD may scatter a conduction electron with spin $\sigma$ from $m = 0$ to $m = 2$, and vice versa. In this respect, the dot acts as an impurity spin $S = 3/2$ in interaction with two channels of conduction electrons (in our case the channel index is the spin index $\sigma = \uparrow, \downarrow$). This would attempt to realize underscreening of the dot’s spin with Kondo temperature $T_{\text{cross}}$. However, if Zeeman spin splitting (ZSS) $\Delta_Z > T_{\text{cross}}$ ($k_B = \hbar = 1$ throughout the paper), two of the dot states are ruled out at temperatures $T$ such that $\Delta_Z > T > T_{\text{cross}}$. The system may flow toward an overscreened $S = \frac{1}{2}$ $2\text{CK}$ fixed point, provided its Kondo temperature $T_{\text{2CK}}$ is such that $T_{\text{2CK}} > T_{\text{cross}}$. (The ZSS should not affect the density of conduction electron states of both spin polarization at $\mu$.)

We now discuss for which values of the parameters the system may exhibit $2\text{CK}$ and estimate the corresponding Kondo temperature (see Fig. 3) by combining exact diagonalization results for an isolated dot with $N = 4, 5, 6$ electrons with scaling approach. We construct the even-parity single-particle states labeled by $q m \sigma$ out of the wavefunctions $e^{i(k_F l m + q)} \phi_{\epsilon, q, m, \sigma}(\rho)$, delocalized in the $z$-direction, with $\epsilon \sim \mu$ and $q \ll k_F l m$ ($k_F l m$ is...
the Fermi wavevector of the 1-d subbands of motion along $z$, labeled by $l$ and linearized about $\mu$). We denote the corresponding operators by $b_{q\mu\sigma}$, $b_{q\mu\sigma}^\dagger$ and drop the energy and subband index for simplicity. The Hamiltonian for the leads is given by $H^b = \sum_{q\mu\sigma} (\epsilon_{q\mu} - \mu) b_{q\mu\sigma}^\dagger b_{q\mu\sigma}$.

Dot states can be expanded in the basis of Slater determinants of single particle orbitals $(n, m)$ associated to the fermion operators $d_{n\mu\sigma}, d_{n\mu\sigma}^\dagger$ (in a in-plane parabolic confining potential, $n = 0, 1, \ldots, n$ and $m = -n, -n+2, \ldots, n-2, n$). In Fig.2 we represent the determinants with $S_z = \frac{1}{2}$ giving the largest contribution to the $N = 4, 5, 6$ GS, by filling a sequence of boxes. $n$ increases by one along the vertical rows of boxes, while $m$ increases along the horizontal rows. A large magnetic field $B$ favors the occupancy of positive $m$ states. All the states have the lowest possible $S_z$, since Hund’s rule does not apply in the presence of a rather strong $B$. The larger is $U$, the higher in energy are $N = 4, 6$-triplet states. Therefore, we neglect virtual transitions to triplets, since $B$ should be cranked up a lot in order to induce transitions to higher spin states of the dot.

Within the subspace $\Xi$, the Hamiltonian of the isolated dot is:

$$H_d = K \sum_\sigma S_\sigma^z + \Delta_Z (P_\uparrow - P_\downarrow)$$

(1)

In Eq.(1), we have introduced the following dot operators:

$$P_{\sigma\sigma'} = \frac{1}{2} \sum_\alpha |5\alpha\sigma\rangle\langle 5\alpha\sigma'|; \quad S^{a}_{\sigma\sigma'} = \frac{1}{2} \sum_{\alpha\alpha'} |5\alpha\sigma\rangle\langle 5\alpha\sigma'|$$

$\alpha$ labels states with different $M$ and $\sigma_{\alpha\alpha'}$ denote the Pauli matrices with $a = 1, 2, 3$. The first term of eq.(1) is a possible detuning of $B$ from $B^\uparrow$, which breaks the degeneracy of the dot states at different $M$ and is ignored in the following. The second term is the ZSS term.

The model hamiltonian for the tunneling between dot and leads is $H_t = \Gamma \sum_{\mu qn\sigma} d_{\mu n\sigma}^\dagger b_{q\mu\sigma}$, $h.c.$ To lowest order in $|\Gamma|^2$, $H_t$ connects dot states $\in \Xi$ to states with $N \pm 1$. At CB, $6E_0 - 5E_0 < \mu < 5E_0 - 4E_0$ and the two most relevant cotunneling processes giving raise to tunneling of the dot between states with $M = 4$ and $M = 6$ are marked by thick solid arrows in Fig.2. The labels $p, h$ refer to whether the lead intermediate state has one extra electron (particle), or one extra hole (hole).

Let us denote the states of the contacts by $|N, \phi\rangle$, where $N$ is the number of electrons and $\phi$ is a collective label for all the appropriate quantum numbers. Generalized magnetization vector operators acting on the contacts at the dot site $z = 0$ in the perturbative $h, p$-process [18] are given by:

$$\tilde{m}_{\alpha\sigma}^p, \tilde{m}_{\alpha\sigma}^h \} = \frac{1}{2} \sum_{\phi\phi'\phi''} \tilde{\rho}_{\alpha\sigma}^{\phi,\phi'} \langle N \mp \{ q\phi\phi'\} |, \phi' \rangle \langle N \pm1 |, \phi' \rangle$$

(2)

Generalized scalar charge density operators, $\tilde{r}_{\alpha\sigma}^{\phi,\phi'}$, are obtained by substituting $\tilde{\rho}_{\alpha\sigma}^{\phi,\phi'}$ with $\delta_{\phi,\phi'}$ in Eq.(3). A Schrieffer-Wolff transformation provides the effective Hamiltonian restricted to the subspace $\Xi$:

$$H_{\text{Eff}} = J \sum_\sigma [P_\sigma \tilde{S}_{\sigma\sigma} + \tilde{S}_{\sigma\sigma} \cdot \tilde{m}_{\sigma\sigma}^p] + J \sum_\sigma [-P_\sigma \tilde{S}_{\sigma\sigma}^h]$$
provides third order scaling equations given by:

\[ + \vec{S}_{\sigma} \cdot \vec{m}_{\sigma} \] + Y \sum_{x=p,h} \sum_{\sigma} \vec{S}_{\sigma} \cdot \vec{m}_{\sigma}^x ; \tag{3} \]

where \( \bar{\sigma} = -\sigma \) and \( J \sim |\Gamma|^2/|E_0 - \mu|, J \sim |\Gamma|^2/|E_0 - \mu| + \mu \).

The dominant \( p \) and \( h \) processes are diagonal in the spin indices and involve only lead electrons with \( \sigma \) opposite or equal to \( S_z \), respectively (see Fig.2). The other possibility corresponds to subleading processes in which the intermediate dot state is a triplet. \( Y \) is the coupling strength for tunneling processes that change both \( M \) and \( S_z \) (off-diagonal terms in the spin labels).

We calculate the couplings in \( H_{\text{Eff}} \) by means of exact numerical diagonalization (Inset of Fig.3). The transverse and longitudinal amplitudes, \( (J^z, J^\perp), (\bar{J}^z, \bar{J}^\perp), (Y^z, Y^\perp) \), are all of the same order of magnitude. Anisotropies between transverse and longitudinal couplings are irrelevant to our argument anyway. Therefore, we assume isotropic magnetic couplings in \( H_{\text{Eff}} \).

\( T > T_{\text{cross}} > \Delta_Z \) case:

A scaling analysis on \( H_{\text{Eff}} \) is performed by rescaling the band cutoff as \( D \rightarrow D - \delta D \) and by working out the corresponding renormalization of the coupling strengths \( J, \bar{J} \) and \( Y \). This provides third order scaling equations given by:

\[
\frac{dJ}{d\ln(D_0)} = \{-\nu(0)[J^2 + Y^2] + \nu^2(0)[J^3 + JY^2]\} ;
\]

\[
\frac{d\bar{J}}{d\ln(D_0)} = \{-\nu(0)[\bar{J}^2 + Y^2] + \nu^2(0)[\bar{J}^3 + \bar{J}Y^2]\} ;
\]

\[
\frac{dY}{d\ln(D_0)} = \{-\nu(0)[JY + \bar{J}Y] + \nu^2(0)[J^2 + \bar{J}^2]Y\} \tag{4}
\]

(\( \nu(0) \) is the density of states at \( \mu \) for each spin polarization).

The initial values of the parameters \( J_0, \bar{J}_0, Y_0 \) define a crossover temperature to strong coupled regime, \( T_{\text{cross}} \). Because of the spin flip term proportional to \( Y \) in Eq.(3), diagonalization of \( H_{\text{Eff}} \) selects one preferred scattering channel, which does not conserve spin and orbital momentum separately. Hence, below \( T_{\text{cross}} \), the system flows towards a 1-channel underscreened strongly-coupled state. Given isotropic couplings, \( J_0 \sim J_0 \sim Y_0 \), \( T_{\text{cross}} = D_0 \sqrt{\nu(0)\bar{J}_0 \exp\left[-\frac{\bar{J}}{2\nu(0)}\right]} \).

\( \Delta_Z \gg T_{\text{cross}} \) case:

Instead, we are interested in the complementary situation, \( \Delta_Z > T > T_{\text{cross}} \). The two \( S_z = -\frac{1}{2} \) dot’s states decouple from the scaling when \( T < \Delta_Z \), and spin-\( \frac{1}{2} \) 2CK may take place in the system. At temperatures below the decoupling point \( H_{\text{Eff}} \) no longer applies. Indeed, the off-diagonal term proportional to \( Y \) in Eq.(3) does not contribute to scaling anymore. As the dot lays within either state with \( S_z = \frac{1}{2}, S_{\uparrow\uparrow} \) becomes a spin-\( \frac{1}{2} \)-operator, \( P_{\uparrow\uparrow} = \frac{1}{2} \), while \( P_{\downarrow\downarrow} = 0 \). The effective Hamiltonian describing low-energy dynamics at the scale \( \Delta_Z \) takes the form of a 2CK-Hamiltonian \( H_{2\text{CK}} \), with the spin index playing the role of the channel index. Coupling constants in \( H_{2\text{CK}} \) are given by the coupling strengths \( J, \bar{J} \) scaled down to \( T = \Delta_Z, J^*, \bar{J}^* \). After a particle-hole transformation is performed in the \( \uparrow \)-spin channel only \((b_{Qm\uparrow} \leftrightarrow (-1)^\bar{m}b_{Qm\downarrow}^\dagger, \) with \( m = 0, 2 \) and \( \bar{m} \neq m \), the Kondo interaction term in \( H_{2\text{CK}} \) is unchanged, while a sign is reversed in the potential part, yielding:

\[
H_{2\text{CK}} = \frac{1}{2} (J^* \rho_{\uparrow\uparrow} + \bar{J}^* \rho_{\downarrow\downarrow} + J^* \bar{S} \cdot \bar{m}_{\uparrow\uparrow} + \bar{J}^* S \cdot \bar{m}_{\downarrow\downarrow} \tag{5} \]
As shown in the inset of Fig.3, fine-tuning of dot’s parameters is possible, to achieve the symmetry condition $J^* = J^*$. Due to the transformation all the virtual processes are all of the same kind and the label $p, h$ has been dropped. The potential scattering in Eq.(5) generates a phase shift responsible for depletion of $p$ states at the Fermi surface. For this reason, it has to be taken into account by diagonalizing it at each step of the renormalization process described by the flow equation:

$$
\frac{dJ^*}{d\ln(\frac{J^*}{T})} = -\nu^p(0)(J^*)^2 + (\nu^p(0))^2(J^*)^3,
$$

(\nu^p(0) is the $p$ density at the Fermi level). From the scaling equation Eq.(5), one derives the corresponding 2CK-temperature: $T_{2CK} = \Delta Z\nu^p(0)J^* e^{-\frac{\nu^p(0)}{\Delta Z}}$. Below, we show that there is a wide range of parameters for which the condition $T_{2CK} > T_{cross}$ is realized. In this case, as $T \to 0$, the system may flow toward a “spin-1/2” 2CK fixed point. Indeed, spin 1/2 2CK takes place if coupling of the two conduction channels is symmetric, $J^* = J^*$. Although this condition is quite demanding, it should be possible to achieve it by properly tuning the gate voltage $V_g$, as shown in the inset of Fig.3. Inclusion of the excited states we neglected in our work ($N = 4, 6$ triplets and so on), will shift the value of $V_g$ corresponding to the symmetry point. The signature of 2CK spin 1/2 fixed point will be in a $\sqrt{T}$ dependence of the conductance below $T_{2CK}$ at a special $V_g$ point, instead of the $T$ behavior, typical of a Fermi liquid fixed point [9](see Fig.1b). In Fig.3 we plot the corresponding relevant temperature scales, $T_{2CK}$ and $T_{cross}$ vs. the hybridization parameter between dot and leads, $\Delta = \nu^p(0)|\Gamma|^2$, in units of the single particle level spacing $\omega_0 = \sqrt{\omega_d^2 + \omega_c^2}/4 = 6$ meV ($\omega_d = 4$ meV is the frequency associated to the confining potential and $\omega_c = 9$ meV is the cyclotron frequency at $B = B^*$). Appropriate choice of the barrier thickness can fix the hybridization parameter $\Delta$ within the required range $\Delta_Z > T_{2CK} > T_{cross}$.

In conclusion, we propose to search for orbital “spin 1/2” 2CK in a QD in a pillar structure, tuned at CB with an odd number of electrons and an appropriate magnetic field along the axis, corresponding to the degeneracy point between GS levels with different values of $M$. Detecting the effect requires an appropriate control of the hybridization of the dot with the contacts and a proper tuning of the gate voltage $V_g$. A measurement of the conductance $G(T)$ vs. $T$ at low temperature will exhibit quadratic behavior and will cross over to a square root behavior, as $V_g$ is tuned so that the two channels become symmetric.

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Fig. 3 – The plot shows $T_{\text{cross}}$, $T_{2CK}$ and the Zeeman spin splitting $\Delta Z$ as a function of the hybridization parameter $\Delta$, according to expressions given in the text. The 2CK conductance may occur when $\Delta Z > T_{2CK} > T_{\text{cross}}$ (hatched area). Values of the parameters are: $\omega_0 = 6$ meV, $D_0 = 30$ meV, $\Delta Z = 1.4$ K, $\nu(0) = 0.084$ meV$^{-1}$. Inset: Plot of the couplings $J_z$ and $\overline{J}_z$ when the position of the dot levels relative to $\mu$ is shifted by changing $V_g$. 

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[14] We understand that we have performed a canonical transformation from the usual basis set, where contact state operators are labeled as e.g. Left (L) and Right (R), to a basis set given by even- and odd-parity linear combinations with respect to the dot’s position. We also assume

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that the dot’s potential is even, so that the two parities decouple, and that the potential itself is strongly localized, so that odd-parity combinations are ruled out.

[15] Contact operators in Eq. (2) cannot be expressed in terms of quadratic combinations of operators $b_{\gamma m\sigma}$ and $b_{\gamma m\sigma}^\dagger$ since ordering in Eq. (2) is fixed.

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