Spin fractionalization of an even number of electrons in a quantum dot

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Kondo resonant conductance can occur in a quantum dot with an even number of electrons $N$ in the Coulomb blockade regime, with bottom and top contacts attached to it in a pillar configuration, in a magnetic field $B_\perp = B^*$ along the axis. The field $B^*$ is tuned at the crossing of levels with different total spins and the spin degeneracy of the dot energies should be lifted. The case of the degeneracy of the singlet-triplet states in a dot with $N = 2$ is analyzed in detail. Coupling to the contacts is antiferromagnetic due to a spin selection rule, so that total spin on the dot is $S = 1/2$ in the Kondo state.

Quantum dots (QD) are remarkable because of Coulomb oscillations. At very low temperature, linear conductance (at vanishing bias $V_{sd}$) is zero, except for peaks at discrete values of the gate voltage $V_g$, when it is energetically favourable to add one extra electron to the dot. Therefore $V_g$ controls the number of particles on the dot in the Coulomb Blockade (CB) regime: its charge is quantized and so is the spin. Dots with an even (odd) number of electrons have integer (half integer) total spin.

However, by lowering the temperature further below some value $T_K$, finite conductance can be found experimentally at zero voltage, relatively insensitive to small changes of $V_g$ within the CB regime, as a mesoscopic realization of the physics of the Kondo effect. The zero voltage anomaly in the conductance is only seen when population is odd. While the charge remains quantized, the spin quantization of the correlated state between the dot and its contacts is changed, due to the formation of a Kondo singlet involving the odd electron.

A weak magnetic field parallel to the dot plane, $B_\parallel$, splits the peaks in the differential conductance into two, located at $V_{sd} = \pm g^* \mu_B B_\parallel$, (where $g^*$ is the effective gioromagnetic factor for electrons in this geometry and $\mu_B = e\hbar/2mc$ is the Bohr magneton), until eventually they disappear.

On the contrary, a magnetic field $B_\perp$, orthogonal to the dot area, is believed to be much more destructive, due to orbital changes of the electron states, in addition to the lifting of spin degeneracy, that prevents the formation of the Kondo correlated state.

We suggest here the possibility that, due to accidental crossing of the lowest non degenerate many body energy levels of the QD at special values of $B_\perp = B^*$, orthogonal to the dot connected to the leads in a pillar structure, the Kondo resonance can still be present, irrespective of the parity of the electron number $N$. In particular we discuss here the case of $N = 2$ and show that under suitable conditions a correlated state sets in, which is characterized by fractionalization of the total spin.

Indeed a QD at high $B_\perp$ (in the $z -$direction) displays a rich level structure that can be monitored attaching bottom and top contacts to it in a pillar structure via linear and non linear transport. Assuming the QD to be effectively two-dimensional and confined by a parabolic potential, its states in isolation can be labelled by the total spin $S$ and the $z -$component of the total angular momentum $M$ and spin $S_z$. In increasing $B_\perp$, many level crossings can occur for an $N$ particle QD between states of increasing $M$, as well as states with higher total spin $S$.

It is well known that the ground state (GS) of an isolated dot with $N = 2$ electrons changes from singlet ($^2S : S = 0, M = 0$) to triplet ($^2T_{S_z} : S = 1, M = 1$) at a value $B_\perp = B^*$, due to crossing of levels $[13]$. Correspondingly, exact diagonalization shows that the $N = 3$ electron dot is in a doublet state ($^2D_{S_z} : S = 1/2, M = 1$ or 2 depending on the field value) (see fig. $[14]$). As shown quantitatively in the following, the dot parameters can be chosen in such a way that $B_\perp$ is high enough to lift spin degeneracy. We take $V_g$ tuned in the CB region between $N = 2$ and $N = 3$ electrons on the dot, and limit our discussion to four states: 1) dot with $N = 1$ in $^1D$, 2-3) dot with $N = 2$ in one of the two degenerate states $^2S_0$, and $^2T_1$, 4) dot with $N = 3$ in $^3D_{1/2}$. Taking only these states allows the mapping of the problem onto the non degenerate Anderson model with the following levels: 1) empty level of zero energy, 2-3) singly occupied level of energy $\epsilon_d$ (doubly degenerate), 4) doubly occupied level of energy $2\epsilon_d + U$. Here $U$ is very large (see below) and, if levels 2-3 and 4 are symmetric with respect to the chemical potential of the contacts $\mu$, what can be controlled by $V_g$, average occupancy of levels 2-3 is $n_d = 1$. This corresponds to $N = 2$ electrons on the dot.

The key observation is the following spin selection rule for the isolated dot $[16]$ : because the $N = 3$ GS for the dot only has $S_z = 1/2$, hybridization of the dot with the contacts can only occur by virtual occupancy of the
dot with an extra spin up electron when the dot is in the \( N = 2 \) singlet state \( ^2S \) or with an extra spin down electron when the dot is in the \( N = 2 \) triplet state with \( S_z = 1 \) \( (^2T_1 \) state). Although spin degeneracy of the dot is assumed to be lifted, the physics is the same as that of the single channel Kondo model with effective spin \( S^{eff} = 1/2 \), in the absence of magnetic field. Here is \( S_z^{eff} = S_z - 1/2 \) and coupling with the delocalized electrons is antiferromagnetic due to the spin selection rule mentioned above. Provided hybridization to the contacts \( \Delta \) is large enough and temperature is below the Kondo temperature \( T_K \), the system flows to the strongly correlated fixed point. Formation of the Kondo singlet corresponds to the confining potential is \( \epsilon_{K} \) and coupling with the delocalized electrons is \( \epsilon_{de} \). Here is the dot, together with a strong zero bias anomaly in the conductance.

In this letter we discuss the properties of the GS, borrowing from the known results of the non degenerate Anderson model \[17\]. In particular, we discuss the spin fractionalization of the total spin of the dot, together with a strong zero bias anomaly in the conductance.

We denote the two dot degenerate energies by \( E_{i} \) \((i = 1 : \) triplet state, \( i = 2 : \) singlet state) and take the chemical potential \( \mu \) of the left and right bulk contacts within the CB valley of the conductance at \( N = 2 \) \((\mu_2 < \mu < \mu_{N+1} = N+1E_N - NE_i)\). Electrons in the contacts are non interacting and have an energy dispersion \( \epsilon_{\sigma} \) involving just one single Landau level and linearized around \( \mu \) with Fermi velocity \( v_F \). The wavevector \( k \) is in the \( z \)-direction and the two contacts are assumed to be equal \((H_{L/R} = \sum_{\kappa \sigma} \epsilon_{\kappa} \sigma b_{L/R, \kappa}^\dagger b_{L/R, \kappa})\) and three dimensional enough, in order to have both spin polarizations at \( \mu \).

The dot Hamiltonian \( H_d \), restricted to the Fock space with \( N = 1, 2, 3 \) electrons can be represented in terms of the occupation numbers \( n_i \) for the degenerate levels \( E_i \):

\[
H_d = \mu_2 \sum_i n_i + U n_1 n_2
\]

where \( U = \mu_3 - 2 \mu_2 \) is the charging energy for adding the third electron to the dot. Here \( n_i = c_i^\dagger c_i \), the vacuum of the \( e \) operators is the dot state with one electron and the \( c_i^\dagger \) create the two degenerate states by acting on it.

The model Hamiltonian is \( H = H_L + H_R + H_d + H_t \), where \( H_t \) is the hybridization term acting only at \( z = 0 \). According to the spin selection rule stated above, it takes the form:

\[
H_t = \frac{1}{\sqrt{2}} \sum_{\kappa} \left\{ \Gamma^\ast_{L/\kappa} (b^\dagger_{L, \kappa} + b^\dagger_{R, \kappa}) c_1 + \Gamma_{L/\kappa}^2 (b_{L, \kappa} + b_{R, \kappa}) \right\} + h.c.
\]

The tunneling amplitudes \( \Gamma_{L/\kappa} \), which depend on the actual features of the device, have been taken all equal for simplicity.

We start integrating out the contacts fields (\( \hbar = 1 \) in the following):

\[
\mathcal{Z}(\mu) \propto \int \Pi_{i} \left( D_{c_i} D_{c_i}^\dagger \right) \exp\left\{-\beta \sum_{\omega} \sum_{\kappa} \Gamma_{\kappa}^\ast \Gamma_{\kappa} (c^\dagger_{1, \kappa} c_{1, \kappa}) \right\}
\]

with

\[
A_{d} = \int_{0}^{\beta} d\tau \left\{ \sum_{i} \left[ c_{i, \uparrow} \frac{\partial}{\partial \tau} c_{i, \uparrow} + \mu_2 \mu \right] \right\} + U c_{1, \downarrow} c_{1, \uparrow} c_{2, \uparrow}
\]

and

\[
K(\omega_m) = \sum_{\kappa} (i\omega_m + \omega k)^{-1}
\]

is taken independent of \( \sigma \) for simplicity. In the limit of large \( U \) we have:

\[
\exp\left[\int_{0}^{\beta} d\tau \left[ U n_1 n_2 - \bar{\mu} (n_1 + n_2) \right] \right]
\]

\[
e^{-\frac{\beta}{U} n_1 n_2 - 2 \bar{\mu} / U} \cdot e^{-\frac{\beta}{U} \int_{0}^{\beta} d\tau (n_1 - n_2)^2}
\]

where the delta function implements the constraint of single site occupancy in the symmetric case, \( \bar{\mu} = \mu - \mu_2 = U/2 \).

We introduce \( X(\tau) \) as an auxiliary boson field coupled to the differential occupancy of the two degenerate states by means of an Hubbard-Stratonovitch decoupling:

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\mathcal{Z}(\mu) \propto \int \Pi_{i} \left( D_{c_i} D_{c_i}^\dagger \right) \exp\left\{-\beta \sum_{\omega} \sum_{\kappa} \Gamma_{\kappa}^\ast \Gamma_{\kappa} (c^\dagger_{1, \kappa} c_{1, \kappa}) \right\}
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We introduce \( X(\tau) \) as an auxiliary boson field coupled to the differential occupancy of the two degenerate states by means of an Hubbard-Stratonovitch decoupling:
the scaling invariant energy is $S_{\alpha} \leq Y \left[19\right]$. Bly degenerate GS of an effective spin 1-dimensional Coulomb gas (CG). We define $U_{\text{eff}} = \frac{\int f_{\alpha}^{\beta} d\tau \cdot X(\tau)^{2} + 2U(n_{1} - n_{2})X(\tau)}{2}$. Then, the partition function of eq.2 reads:

$$Z(\mu) \propto \int DX e^{-\frac{1}{\beta} \int f_{\alpha}^{\beta} d\tau X(\tau)} \times \Pi \left(D_{c}, D_{c}^{+} \right) e^{-\int^{\beta} \int f_{\alpha}^{\beta} d\tau X(\tau)} \times \delta(n_{1} + n_{2} - 1) \sum_{j=1}^{2} e^{-\frac{1}{2} \int f_{\alpha}^{\beta} d\tau n_{j}} = 2 \left[1 + \frac{1}{\beta} \right] \left(\frac{\lambda_{\text{eff}}}{\lambda_{\text{eff}} + 1}\right)^{2} \sim S_{\alpha} \leq Y \left[19\right] \left(\frac{\lambda_{\text{eff}}}{\lambda_{\text{eff}} + 1}\right)^{2} \sim U/2.$$

(3)

where is $G_{(0)}^{(-1)}(i\omega_{m}) = i\omega_{m} + [\Gamma]^2 K(i\omega_{m})$. We will take the saddle point solution of eq.8 quite closely, to map eq.2 on a 1-dimensional Coulomb gas (CG). We define $\xi(\tau) = X(\tau) / \Delta$, where $\Delta = 2\pi N(0)\Gamma^2$ and $N(0) = L/\pi \nu_{F}$ ($L$ is the size of each single contact) is the density of states at the Fermi energy. At low temperatures, saddle point solutions of the resulting single particle effective action are sequences of instantons $\xi_{l}(\tau, t) = \pm \xi_{0} \tanh((\tau - t_{l})/\tau_{0})$ ($t_{l}$ are the centers, $l = 1, 2, \ldots$) corresponding to jumps between the two minima of the effective potential, $V[\xi] = \Delta^{2}/U \xi^{2} - 2\Delta / \pi \xi^{2} \xi^{-1} + \frac{1}{2} \ln(1 + \xi^{2}) \left[19\right]$, located at $\xi_{0} = \pm \Delta / 2\Delta$, that interact via a logarithmic potential $\alpha^{2} \ln |t_{i} - t_{j}| / \tau_{0}$. The bare strength of the logarithmic interaction is $\alpha^{2} = 2(1 - 4\Delta / U \pi^{2})$. The bare fugacity of the CG is $Y_{0} = \tau_{0} \exp(-\bar{A})$ ($\bar{A} \sim \tau_{0} U$ is the action of one single blip). The scaling of the fugacity and the renormalization of the coupling constant induced by processes of fusion of charges lead to the Renormalization Group (RG) equations $\left[22\right]$. 

$$\frac{dY}{d\ln \tau_{0}} = 1 - \alpha^{2} Y, \quad \frac{d\alpha^{2}}{d\ln \tau_{0}} = -2Y^{2} \alpha^{2} \left(4\right)$$

The flow is towards $Y \to \infty$ and $\alpha^{2} \to 0$, and the scaling invariant energy is $T_{K} = \tau_{0}^{-1} e^{1/(1 - 2\Delta)} \sim (U\Delta)^{2} e^{-\pi^{2} U/(4\Delta)}$. Condensation of instantons in the doubly degenerate GS leads to the Kondo singlet $<S^{\text{eff}} > = 0$ or $<S > = \frac{1}{2}$ on the dot.

An heuristic argument for the fractionalization of the total spin $S$ of the dot reads as follows.

The dynamics of the field $\xi(\tau)$ of action $\bar{A}$ can be mimicked by a two level system hamiltonian $H_{2L}$ with hopping energy $\lambda \sim \frac{1}{2}m_{c}^{*}f_{\alpha}^{\beta} \left(\frac{d\xi}{d\tau}\right)^{2} \sim \frac{1}{2}(\Delta^{2} - \tau_{0}^{2})^{2} \sim U/2.$ The role of the interaction is to project out higher energy components from the dot states. Denoting by $|\pm >$ the two eigenstates of $H_{2L}$, the dynamics of the dot is between states $\Pi^{0}|S > /N_{\alpha}^{2} (g)$ and $\Pi^{0}|T > /N_{\alpha}^{2} (g)$, where $<S >$ and $<T >$ are the states localized in the two potential wells and $N_{S/T}(g)$ are their normalizations. $\Pi = 1 - g\Pi_{0}$ is the Gutzwiller operator partly eliminating the component on the high energy eigenstate $|\pm > (g \in (0,1)) \left[22\right].$

Now we state the connection with the CG picture given above. The frequency $\lambda/2\pi$ is obviously related to the average number of flips: $\beta\lambda/2\pi = < N > / \tan Y$ and probability of having the system in states $|\pm >$ at temperature $\beta^{-1}$ are

$$P_{-} = \frac{e^{-\pi Y / 2} 1 + 4\pi^{2} Y^{2}}{1 + e^{-4\pi Y / 2} Y^{2}}; \quad P_{+} = \frac{1}{1 + e^{-4\pi Y / 2} Y^{2}} \left(5\right).$$

Equating these probabilities to the ones given by $P_{+} = < |+ > / < \Pi | S > / T > ^{2} / N_{S/T}(g)$ yields the correspondence $1 - g \to e^{-2\pi Y / 2} Y$. The $z-$ component of the total spin of the projected singlet and triplet state are given by

$$< S_{z} >_{S,T} = \frac{g}{2} \left(1 - \frac{1}{1 + g^{2}}\right); \quad < S_{z} >_{S,T} = \frac{1}{2} \left(\frac{1}{1 + g^{2}}\right) \left(4\right).$$

Because $Y$ scales to infinity, $g \to 1$: the higher energy state completely decouples and $< S_{z} >_{S,T} \to \frac{1}{2}$. We now give some estimates for a possible practical realization.

If the level separation of the parabolic confining potential of the dot is $h\omega_{c} = 4m eV$, the effective frequency in presence of $B_{\perp}$ is $\omega_{l} = \sqrt{\omega_{l}^{2} + \omega_{c}^{2} / 4} \left(19\right)$. The Coulomb interaction between electrons in the plane is $E_{c} \times l_{0}/|\vec{r} - \vec{r}'| \left(19\right)$ where $E_{c} = 3m eV$ and $l_{0}^{2} = h/m^{*} \omega_{c}$). This choice of the parameters gives a singlet-triplet (S-T) transition for the dot with $N = 2$ at $B_{\perp} = B^{*} \approx 4.5$ Tesla, close to one of the Delft experiments $\left[22\right]$. Fig.7 shows the total energy of the dot vs magnetic field for $N = 2$ and $N = 3$. Zeeman spin splitting of the energies is not included in the picture for clarity, although it is sizeable at these fields: $g_{\mu B} \mu B = 0.11 m eV$. Here we assume the bulk gromagnetic factor for GaAs $g_{\mu} = -0.44$, but it could be lower $\left[22,23\right]$. In any case, at temperatures below $300 m K$ the spin degeneracy is lifted. According to fig.7 the energy difference between the GS’s when three and two electrons are on the dot is $U = 3 \left(2 - 2 E = 12.5 m eV \right)$ at the S-T crossing, which is about 1/3 higher than the value
\[ E_c + \hbar \omega_0 = 3.0 \text{meV} + 5.55 \text{meV} \] predicted by a constant interaction model. The \( N = 3 \) particle state is a doublet (\( S = 1/2 \)) \( 3D \) with \( M = 1 \). Higher magnetic fields produce its crossing with the doublet with \( M = 2 \), while, increasing \( B_\perp \) further, the quadruplet state (\( Q : S = 3/2 \)) becomes lower in energy.

The order of magnitude of the hybridization of the dot with the contacts \( \Delta \) is fixed by the requirement that neighbouring CB peaks in the conductance do not overlap \( [3] \). Their separation is \( \sim \hbar \omega_0 \). For values of \( \Delta \sim (0.1 - 0.2) \hbar \omega_0 \), \( T_K \) (given below) is of tenths of \( mK \). We have neglected the excited states of the two particle dot in the description. This is allowed because \( T_K \) is much less than the spin splitting of energy levels.

The next available state in the spectrum of the isolated dot with \( N = 2 \) is the triplet state with \( S_z = 0 \) (\( 2T_0 \)). Because it is non degenerate, no Kondo-like coupling is possible. This state can only hybridize with conduction electrons via cotunneling processes which, in the classical case, give rise to currents that are linear in the biasing voltage \( V_{sd} \) and of the order of \( \sim (\Delta^2/U) V_{sd} \).

We conclude that the problem is equivalent to a non degenerate Anderson model in absence of magnetic field. At \( B_\perp = b^* \), the \( N = 2 \) particle dot can be in the \( 2S_0 \) or \( 2T_1 \) state, but addition of one more electron requires an extra energy \( U \). Furthermore is \( U \gg \Delta \). The results are expected to be quite robust with respect to small changes of the magnetic field away from \( B^* \), especially for \( B_\perp < B^* \) because the reference field \( H_0 = (U \Delta) / \mu_B \) is of the order of Tesla. For \( B_\perp > B^* \), instead, the state \( 2T_1 \) will be eventually favoured in energy.

A small a.c. magnetic field \( |B_\parallel| \ll |\delta B| \sim T_K/\mu_B \) (with \( \delta B = B_\parallel - B^* < 0 \)) could induce transitions between the two degenerate Kondo GS’s, with Rabi frequency \( \hbar \omega_R = M_\Delta |\delta B| \). The quantity \( M_\Delta/2 \approx \frac{g_s \mu_B}{2} \left[ 1 + \delta B/(\pi T_K) \right] \) is the expected magnetic moment of the Dot with \( N = 2 \), in the Kondo state. The measurement, if feasible, should be performed just off \( B_\parallel = b^* \) for \( \delta B < 0 \), not to match the energy separation of the two levels \( 2T_1 \) and \( 2T_0 \).

In conclusion, we have discussed the possibility that the total spin state of a dot in CB with \( N = 2 \) is strongly coupled to the spins of the electrons in the leads. This kind of mesoscopic Kondo effect would give rise to fractionalization of S in the dot, i.e. to a sort of ‘spinon box’.

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