Kondo screening of a high-spin Nagaoka state in a triangular quantum dot

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Abstract

We study transport through a triangle triple quantum dot connected to two noninteracting leads using the numerical renormalization group (NRG). The triangle has a high-spin ground state of \( S = 1 \) caused by a Nagaoka ferromagnetism, when it is isolated and has one extra electron introduced into a half-filling. The results show that the conduction electrons screen the local moment via two separate stages with different energy scales. The half of the \( S = 1 \) is screened first by one of the channel degrees, and then at very low temperature the remaining half is fully screened to form a Kondo singlet. The transport is determined by two phase shifts for quasi-particles with even and odd parities, and then a two-terminal conductance in the series configuration is suppressed \( g_{\text{series}} \approx 0 \), while plateau of a four-terminal parallel conductance reaches a Unitary limit value \( g_{\text{parallel}} \approx 4e^2/h \) of two conducting modes.

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The Kondo effect in quantum dots is an active field of current research, and recently triple quantum dots with triangle have been examined intensively [1,2].

One interesting property expected to be seen in a quantum-dot array with closed paths is that some degenerate states could be lifted by circular orbital motions of electrons to form a high-spin ground state due to the Nagaoka mechanism. In this report for clarifying, i) how the Nagaoka ferromagnetism that could manifest in the isolated triangle for a particular charge filling is screened by the conduction electrons, and ii) how it affects the low-temperature transport bellow the Kondo energy scale \( T \lesssim T_K \).

We start with a three-site Hubbard model connected to two non-interacting leads on the left(\( L \)) and right(\( R \)), as shown in Fig. 1 (a): \( \mathcal{H} = \mathcal{H}_D + \mathcal{H}_{\text{mix}} + \mathcal{H}_{\text{lead}} \).

\[
\mathcal{H}_D = -t \sum_{<ij>, \sigma}^N_D \left( d_{i\sigma}^\dagger d_{j\sigma} + d_{j\sigma}^\dagger d_{i\sigma} \right) + \epsilon_d \sum_{i=1}^N_D d_{i\sigma}^\dagger d_{i\sigma} + U \sum_{i=1}^N_D d_{i\uparrow}^\dagger d_{i\downarrow} d_{i\downarrow}^\dagger d_{i\uparrow} ,
\]

\[
\mathcal{H}_{\text{mix}} = v \sum_{\sigma} \left( d_{1\sigma}^\dagger \psi_{L\sigma} + d_{N_D\sigma}^\dagger \psi_{R\sigma} + \text{H.c.} \right) ,
\]

\[
\mathcal{H}_{\text{lead}} = \sum_{\nu=L,R} \sum_{k\sigma} \epsilon_{\nu\sigma} c_{\nu\sigma}^\dagger c_{\nu\sigma} ,
\]

where \( t \) is the hopping matrix element between the dots, \( \epsilon_d \) the onsite energy, \( U \) the Coulomb interaction, and \( N_D = 3 \). A linear combination of the conduction electrons \( \psi_{\nu\sigma} \equiv \sum_k c_{\nu\sigma k} / \sqrt{N} \) hybridizes with the electrons in the dots via \( v \), or \( \Gamma \equiv \pi v^2 \rho \), where \( \rho \) is the density of states for each lead. The low-energy states of the whole system including the leads show a local Fermi-liquid behavior, which is characterized by two phase shifts \( \delta_{\text{even}} \) and \( \delta_{\text{odd}} \) for the quasi-particles with the even and odd parities. Then the dc conductance \( g_{\text{series}} \) and total number of electrons in the dots \( N_{\text{el}} \) can be expressed at \( T = 0 \) in the form [3,4],

\[
g_{\text{series}} = \frac{2e^2}{h} \sin^2 \left( \delta_{\text{even}} - \delta_{\text{odd}} \right) ,
\]
both of the two conducting modes contribute to the plateau $g - \delta$ values $\epsilon_{\text{trons}}$ occupy the degeneracy and makes a

$$N_{\text{el}} \equiv \sum_{i=1}^{N_{\text{el}}} \left( \langle d_i^\dagger d_i \rangle - \frac{2}{\pi} \left( \delta_{\text{even}} + \delta_{\text{odd}} \right) \right).$$

Furthermore, because of some symmetrical reasons, the conductance for the current flowing in the horizontal direction in a four-terminal geometry, as shown in Fig. 1 (b), can be related to these two phase shifts defined with respect to the series connection $[3, 4]$

$$g_{\text{parallel}} = \frac{2e^2}{h} \left( \sin^2 \delta_{\text{even}} + \sin^2 \delta_{\text{odd}} \right).$$

We have deduced $\delta_{\text{even}}$ and $\delta_{\text{odd}}$ from the fixed-point eigenvalues of the discretized Hamiltonian $H_N$ of NRG.

In Fig. 2, the results of $g_{\text{series}}$, $g_{\text{parallel}}$ and $N_{\text{el}}$ are plotted as functions of $\epsilon_d$ that corresponds to the gate voltage. The number of electrons inside the triangle increases with decreasing $\epsilon_d$ showing a staircase behavior at $N_{\text{el}} \simeq 1, 2, 3, 4$, and 6. Due to a degeneracy arising in the ground state at $\epsilon_d/U \simeq -1.15$, the average charge changes directly from 4 to 6 without taking a step corresponding to $N_{\text{el}} \simeq 5$. We see that the conductances for small filling $\epsilon_d/U \gtrsim -0.8$ show the typical Kondo behavior, which has also been seen in a linear chain of quantum dots $[3, 4]$. Namely, for odd occupancies $N_{\text{el}} \simeq 1$ and 3, the plateaus of $g_{\text{series}}$ and $g_{\text{parallel}}$ reach the Unitary-limit value $2e^2/h$ of a single conduction mode. We also found a very narrow dip of $g_{\text{series}}$ at $\epsilon_d/U \simeq -0.6$. For an even occupancy at $N_{\text{el}} \simeq 2$, the conductances are suppressed. The irregular behavior at $N_{\text{el}} \simeq 4$ is partly relating to the fact that, for $U = 0$, the circular motion along the triangle forms two degenerate orbitals at $\epsilon_o \equiv t$ and a single orbital at $\epsilon_o \equiv -2t$. As two of the four electrons occupy the $\epsilon_o$ orbitals, the Coulomb repulsion lifts the degeneracy and makes a $S = 1$ state to be a many-body ground state for $\Gamma = 0$. This corresponds to the Nagaoka state, and also links to a flat-band ferromagnetism.

Then, the conduction electrons from the leads screen the $g_{\text{series}}$ and $g_{\text{parallel}}$ are suppressed. The irregular behavior at $N_{\text{el}} \simeq 2$ contributes to the plateau of $g_{\text{parallel}} \simeq 4e^2/h$ at $T = 0$. The difference between the peak values of the two conductances itself is caused by an interference effect.

In order to give some insights into the screening mechanism of the $S = 1$ moment, the low-lying energy levels of the NRG version of Hamiltonian $H_N$ are plotted against odd $N$ in Fig. 3. The trajectory of the levels shows how the system evolves from the high-energy regime to the low-energy Fermi-liquid regime as $N$ increases, or equivalently with decreasing energy $\omega_N \sim D\Lambda^{-N(N-1)/2}$, where $D$ is the half-width of the conduction bands and $\Lambda$ is the parameter for the logarithmic discretization. Our results indicate clearly that two crossovers occur separately at $N \simeq 20$ and $N \simeq 80$. This feature and additional information about the total spin and electron number of the eigenstates show that at high temperatures $T \gtrsim \omega_N=20$ the $S = 1$ moment is free from the screening. Then at the intermediate temperatures, $\omega_N=80 \lesssim T \lesssim \omega_N=20$, the half of the moment is screened by the conduction electrons from one of the channel degrees, and thus in this region the local moment is still in an under-screened situation. The full screening is completed finally at very low temperatures $T \lesssim \omega_N=80$.

The competition between the Kondo effect and Nagaoka ferromagnetism could happen in a wide of class of quantum dots that have closed paths for the orbital motion.

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References

[1] A. Vidan, R. M. Westervelt, M. Stopa, M. Hanson and A. C. Gossard, Appl. Phys. Lett. 85, (2004), p. 3602.
[2] T. Kuzmenko, K. Kikoin and Y. Avishai, Phys. Rev. Lett. 96, (2006), p. 046601.
[3] Y. Nisikawa and A. Oguri, Phys. Rev. B 73, (2006), p. 125108.
[4] A. Oguri, Y. Nisikawa and A. C. Hewson: J. Phys. Soc. Jpn. 74 (2005), p. 2554.
[5] A. Oguri and A. C. Hewson: J. Phys. Soc. Jpn. 74 (2005), p. 988.