Gate-voltage dependence of Kondo effect in a triangular quantum dot

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Abstract. We study the conductance through a triangular triple quantum dot, which are connected to two noninteracting leads, using the numerical renormalization group (NRG). It is found that the system shows a variety of Kondo effects depending on the filling of the triangle. The SU(4) Kondo effect occurs at half-filling, and a sharp conductance dip due to a phase lapse appears in the gate-voltage dependence. Furthermore, when four electrons occupy the three sites on average, a local $S=1$ moment, which is caused by the Nagaoka mechanism, is induced along the triangle. The temperature dependence of the entropy and spin susceptibility of the triangle shows that this moment is screened by the conduction electrons via two separate stages at different temperatures. The two-terminal and four-terminal conductances show a clear difference at the gate voltages, where the SU(4) or the $S=1$ Kondo effects occurring.

1. Introduction
The Kondo effect in quantum dots has been studied in various kinds of systems in recent years, and the triple quantum dots with a triangular configuration is one of the interesting systems [1,2]. Specifically, the closed path along the triangle causes a high-spin ground state with the Nagaoka mechanism [3], and also an SU(4) Kondo effect, depending on the gate voltage. In this report we study the triangular triple dot connected to two noninteracting leads, and present the results of the scattering phase shifts obtained with the numerical renormalization group (NRG). We also calculate the temperature dependence of the entropy and spin susceptibility [4], which show clearly the two-stage screening process of the high-spin Nagaoka state and also the feature of the Kondo screening in the SU(4) case at half-filling.

2. Model & Formulation
We consider a three-site Hubbard model on a triangle, which is connected to two non-interacting leads on the left ($L$) and right ($R$), at $i = 1$ and $i = N_D$ ($\equiv 3$), respectively, as shown in Fig. 1 (a). The total Hamiltonian has the form $\mathcal{H} = \mathcal{H}_D + \mathcal{H}_{\text{mix}} + \mathcal{H}_{\text{lead}}$, with

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

$$\mathcal{H}_{\text{mix}} = v \sum_{\sigma} \left( d_1^\dagger \sigma C_{L\sigma} + d_3^\dagger N_D,\sigma C_{R\sigma} + \text{H.c.} \right) ,$$

$$\mathcal{H}_{\text{lead}} = \sum_{\nu=L,R} \sum_{k\sigma} \epsilon_k c_{k\nu}^\dagger c_{k\nu} ,$$
Here, $t > 0$ is the hopping matrix element between the dots, $\epsilon_d$ the onsite energy in the dots, and $U$ the Coulomb interaction. The conduction electrons around the dots, $C_{\nu \sigma} \equiv \sum_k \epsilon_{k\nu\sigma}/\sqrt{N}$, can tunnel into the triangle via $v$, and it causes the level broadening $\Gamma \equiv \pi \rho v^2$ with $\rho$ the density of states of the leads. In the limit of $v = 0$ and $U = 0$, the circular motion along the triangle forms a single orbital at $E_n \equiv -2t + \epsilon_d$ and two degenerate orbitals at $E_b \equiv t + \epsilon_d$. This degeneracy brings interesting varieties to the Kondo effect, occurring in the triangular quantum dot at different values of $\epsilon_d$, which can be controlled by the gate voltage.

The low-energy states of the whole system including the leads show a local Fermi-liquid behavior, which is characterized by the two phase shifts, $\delta_e$ and $\delta_o$, for the quasi-particles with the even and odd parities. Specifically, at $T = 0$, the conductance $g_{el}$ and the local charge $N_{el}$ in the triangle can be expressed, respectively, in the Landauer and Friedel-sum-rule forms [5],

$$g_{el} = \frac{2e^2}{h} \sin^2 (\delta_e - \delta_o) , \quad N_{tot} \equiv \sum_{i=1}^{N_D} \sum_\sigma \langle d_{i\sigma}^\dagger d_{i\sigma} \rangle = \frac{2}{\pi} (\delta_e + \delta_o) . \quad (3)$$

Owing to an inversion symmetry, the conductance $g_p$ for the current flowing along the horizontal direction in a four-terminal geometry, shown in Fig. 1 (b), can also be obtained from these two phase shifts defined with respect to the two-channel model $\mathcal{H}$, as $g_p = (2e^2/h) (\sin^2 \delta_e + \sin^2 \delta_o)$. We have deduced the value of $\delta_e$ and $\delta_o$ from the fixed point of NRG [5–7]. Furthermore, the quantum dots contribution of the free energy $F_D$ may be defined by [4],

$$F_D \equiv F - F_{lead} , \quad e^{-F/T} = \text{Tr} e^{-H/T} , \quad e^{-F_{lead}/T} = \text{Tr} e^{-H_{lead}/T} . \quad (4)$$

One can also calculate the entropy $S \equiv -\partial F_D/(\partial T)$ and spin susceptibility $\chi \equiv -\partial^2 F_D/(\partial H^2)$. Here, the magnetic field $H$ is introduced by replacing the energy levels $\epsilon_d$ and $\epsilon_k$, respectively, by $\epsilon_{d\sigma} \equiv \epsilon_d - (H/2) \text{sgn} \sigma$ and $\epsilon_{k\sigma} \equiv \epsilon_k - (H/2) \text{sgn} \sigma$.

3. NRG results

In Fig. 2, the results of (a) the phase shifts $\delta_e$, $\delta_o$ and local charge $N_{el}$, and (b) the conductances $g_e$ and $g_o$, are plotted as functions of $\epsilon_d$. The number of electrons in the triangle $N_{el}$ increases with decreasing $\epsilon_d$, showing the steps for $N_{tot} \simeq 1, 2, 3, 4$, and 6. It changes directly from $N_{el} \simeq 4$ to $N_{el} \simeq 6$ at $\epsilon_d \simeq -1.15U$ without taking the step for $N_{tot} \simeq 5$. This is caused by a property of the triangle: the ground state degenerates for the three charge states $N_{tot} = 4, 5$, and 6 at $\epsilon_d \simeq -1.15U$ in the isolated limit $\Gamma = 0$. The Coulomb repulsion lifts partly the degeneracy due to the orbitals with the energy $E_b$. Specifically at the filling $N_{el} \simeq 4$, a high-spin $S = 1$ state becomes the ground state for $U > 0$ by the Nagaoka mechanism for the ferromagnetism. For finite $\Gamma$, the conduction electrons tunneling from the two leads screen the $S = 1$ moment at low temperatures to form a Kondo singlet. The series and parallel conductances through the singlet ground state show a clear difference in this region $-1.15 \lesssim \epsilon_d/U \lesssim -0.83$, as seen in Fig. 2 (b). We see that both of the partial waves contribute to the parallel conductance to give the
plateau of \( g_p \simeq 4e^2/h \), while the series conductance is suppressed \( g_s \simeq 0 \) by the interference. Correspondingly, the phase shifts take the values \( \delta_e \simeq 3\pi/2 \) and \( \delta_o \simeq \pi/2 \).

For small values of the electron occupancies \( N_{\text{tot}} \lesssim 2.0 \), seen at \(-0.3 \lesssim \epsilon_d/U \), the phase shift \( \delta_e \) for the even-parity partial wave increases for decreasing \( \epsilon_d \), while the odd one is almost zero \( \delta_o \simeq 0 \). It implies that in this region the electrons occupy mainly the orbital of \( E_o \) that has an even parity, although generally each phase shift does not necessary correspond to the occupancy of the eigenstates with the same parity. Nevertheless we have confirmed, by calculating directly the occupation number of the each the partial waves \( N_{\text{even}} \) and \( N_{\text{odd}} \) which satisfies \( N_{\text{tot}} = N_{\text{even}} + N_{\text{odd}} \), that an approximate relation \( N_{\text{even}} \simeq 2\delta_e/\pi \) holds well for each partial wave in the two regions, \( \epsilon_d/U \lesssim -0.85 \) and \(-0.6 \lesssim \epsilon_d/U \). However, such a separation of the Friedel sum rule does not hold for the intermediate region \(-0.85 \lesssim \epsilon_d/U \lesssim -0.6 \): while each phase shift takes a constant value \( 2\delta_e/\pi \simeq 3.0 \) and \( 2\delta_o/\pi \simeq 0.0 \), the occupation calculated directly has a different constant \( N_{\text{even}} \simeq 2.5 \) and \( N_{\text{odd}} \simeq 0.5 \). These values suggest that, after two electrons occupy the orbital of the energy \( E_o \), the third electron occupies the degenerate orbitals of the energy \( E_b \) in equal weights. Although the coupling with the two leads breaks the full triangular symmetry of the conduction bands, it seems as if the charge distribution recovers effectively the degeneracy at \( \epsilon_d \simeq -0.6U \). During the sudden change of the phase shifts at \( \epsilon_d \simeq -0.6U \), the sum \( \delta_e + \delta_o \simeq 3\pi/2 \) and the parallel conductance \( g_p \simeq 2e^2/h \) change their values very little. On the other hand, the phase difference \( \delta_e - \delta_o \), varies rapidly from \( \pi/2 \) to \( 3\pi/2 \). This rapid and continuous change of \( \delta_e - \delta_o \) causes the narrow dip observed for the series conductance \( g_s \) at \( \epsilon_d \simeq -0.6U \) in the middle of the conductance plateau. The dip is also related to the SU(4) symmetry. In contrast, the conductance at \( N_{\text{tot}} \simeq 1 \) is caused by the usual SU(2) Kondo effect due to \( S = 1/2 \) moment.

In Fig. 3 (a) the temperature dependence of the entropy \( S \) and \( 4\chi T \), which are obtained at \( \epsilon_d = -1.01U \) in the middle of the charge step for \( N_{\text{tot}} \approx 4 \), is plotted as a function of \( \log(T/D) \), where \( D \) is the half-width of the conduction bands. The results clearly show that the screening of the spin \( S = 1 \) local moment due to the Nagaoka mechanism occurs via two separate stages at \( T/D \simeq 10^{-10} \) and \( T/D \simeq 10^{-30} \). We see that the entropy takes the value \( S \simeq \log 3 \) at high temperatures for \( T/D \gtrsim 10^{-7} \), and it means that the \( S = 1 \) moment is free. Then, at intermediate temperature \( 10^{-28} \lesssim T/D \lesssim 10^{-10} \), the entropy becomes \( S \simeq \log 2 \). It shows that

![Figure 2](image-url)
the half of the moment is screened by the conduction electrons from one of the channel degrees, and the local moment is still in an under-screened state. The full screening is completed finally at very low temperatures $T/D \lesssim 10^{-30}$, as we can see also in the behavior of $\chi$.

Similarly, the entropy and the spin susceptibility for $\epsilon_{sd} = -0.59U$, just at the dip of $g_s$ for $N_{tot} \simeq 3$, are plotted in Fig. 3 (b). At the high temperatures $T/D \gtrsim 10^{-6}$, the entropy takes a constant value $S \simeq \log 4$, which implies that there exist four degenerate local states at the triangle. The screening completes at $T/D \simeq 10^{-8}$, and it may be regarded as the SU(4) Kondo effect. We see that the spin susceptibility for $T/D \gtrsim 10^{-4}$ shows the Curie behavior $\chi \simeq S(S + 1)/(3T)$ with the coefficient corresponding to $S = 1/2$. Therefore the degenerate states have the spin $S = 1/2$ degrees of freedom, and thus the remaining degrees of freedoms of the four fold degeneracy should have an orbital origin in the triangle.

4. Summary
We have studied the ground state properties of a triangular triple quantum dot connected to two noninteracting leads, and have found that the system shows the SU(4) and the $S = 1$ two-stage Kondo effects, as well as the usual SU(2) one, depending on the gate voltage $\epsilon_{sd}$.

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