SU(3) Kondo effect in spinless triple quantum dots

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We discuss a device — a purely capacitively coupled interacting spinless triple quantum dot system — for the observation of the SU(3) Kondo effect. Unlike more familiar SU(2) and SU(4) Kondo effects in quantum dot devices which lead to unitary linear conductance at low temperatures, the SU(3) Kondo scenario can be easily identified by the conductance pinned to a characteristic value of 3/4 of the unitary limit. This is associated with the interesting fact that the SU(3) Kondo effect does not occur at the particle-hole symmetric point, where the system is found instead in the valence-fluctuating regime with the total dot occupancy fluctuating between 1 and 2, but for gate voltages in the two Kondo plateaux where the dot occupancy is pinned to an integer value, either 1 or 2. From the thermodynamic analysis in the Kondo regime we find that the effective impurity orbital moment, defined through the impurity orbital susceptibility ($\chi_{\text{imp}}$) multiplied by the temperature, is $T_{\chi_{\text{imp}}} = 1$ at high temperatures and then it increases to the characteristic value of $T_{\chi_{\text{imp}}} = 4/3$ corresponding to the three-fold degenerate local-moment fixed point where the impurity entropy is $S_{\text{imp}} = \ln 3$. Then, at much lower temperatures, the system flows to the non-degenerate strong-coupling fixed point in which the SU(3) Kondo effect takes place. We also report results about the robustness of the SU(3) Kondo effect against various perturbations present in real experimental setups, namely, unequal reservoir-dot tunneling couplings, gating effects and non-vanishing interdot tunneling rates. Finally, we describe possible mechanisms to restore the SU(3) Kondo physics by properly tuning the on-site dot potentials. We briefly comment on the spinfull case which has very different behavior and shows Kondo plateaus in conductance for all integer values of the occupancy, including at the particle-hole symmetric point.

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I. INTRODUCTION

In metals, magnetic impurities are responsible for the anomalous behavior of the resistivity at low temperatures. Magnetic interactions result from high-order correlated tunneling events of electrons that are hopping in and out of a localized impurity. In this fashion, the impurity spin is screened through the formation of the Kondo spin singlet state. In semiconductor quantum dots, the Kondo effect can also take place as theoretically predicted and experimentally observed. However, whereas the resistivity of a magnetically doped metal increases when the temperature is lowered below the Kondo temperature, $T_K$, in quantum dots (QDs) the linear conductance increases and eventually reaches its maximum value $G = 2e^2/h$ at zero temperature. This is due to the enhancement of the scattering rate which results in the opening of a channel for electrons that are perfectly transmitted through the QD. The main advantage of exploring the spin-1/2 Kondo effect in manufactured nanostructures such as QDs is their high tunability. Using gate electrodes it is possible to vary in a controllable manner the number of trapped electrons and the strength of tunnel coupling between the reservoirs and the localized dot states. Furthermore, as an additional advantage, we mention that QDs constitute perfect laboratories to test many-body effects under non-equilibrium conditions. The influence of external fields such as finite bias voltages or time varying dc fields allows the observation of the Kondo effect out of equilibrium. Remarkably, magnetic fields dramatically affect the Kondo state, even at equilibrium conditions. The level degeneracy, required for the formation of the usual spin-1/2 Kondo effect, is lifted in the presence of a magnetic field. There are, however, some exceptions where a magnetic field facilitates the development of a Kondo state, for example in vertical QDs with an even number of electrons. Here, the integer-spin Kondo effect occurs when the singlet and triplet states become degenerate because of the presence of the magnetic field. Therefore, in general, magnetic fields either remove the Kondo effect or facilitate its observation through the level degeneracy requirement.

The fabrication of more complex nanostructures has opened new possibilities for the study of unconventional Kondo effect. There exists a great variety of artificially fabricated systems exhibiting exotic kinds of the Kondo effect: to mention just a few, nanodevices based on carbon materials like fullerenes, carbon nanotubes, and graphene. Others systems, such as p-doped nanowires, have demonstrated the Kondo effect assisted by holes. The search for highly symmetric Kondo singlets has been revived in carbon nanotubes and vertical double dot systems with the experimental demonstration of the SU(4) Kondo effect. In carbon nanotubes, the valley isospin together with the spin degree of freedom manifests as a four-fold shell structure in the Coulomb blockade regime. In the low-temperature regime the fluctuations among the four quantum states lead to the observation of the SU(4) Kondo effect. So far, the SU(2) and SU(4) Kondo effects have been extensively studied. There is, however, very few works devoted to other possible symmetries for a Kondo singlet, and in particular to the SU(3) Kondo effect.
In a recent work, the SU(3) Kondo effect has been suggested to be observable in triple quantum dot (TQD) in the quantum Hall regime. Here, we discuss a different setup—a spinless TQD with equal capacitative coupling $V_i$ between all quantum dot pairs, as shown in the sketch in Fig. [1] as a suitable system for the observation of the SU(3) Kondo effect. The SU(3) Kondo physics takes place when there is a single electron or a single hole in the whole system, i.e., when either $n = 1$ (one electron and two holes) or $n = 2$ (two electrons and one hole). This defines three possible flavors corresponding to the position of the electron (or hole) in one of the three dots or leads. In this work, we will refer to the flavor degree of freedom also as the channel or orbital degree of freedom; for our spinless model, these expressions are fully interchangeable. Each dot is connected to two contacts in such a way that the tunneling events conserve the flavor degree of freedom. Notice that in principle, this setup can be easily generalized to build an arbitrary SU($N$) Kondo state, although that would entail designing a device with equal capacitive coupling between all QD pairs. Importantly, the only interaction among the dots is capacitative and there is no particle exchange from one dot to the others, i.e., the interdot tunneling is not allowed since this would destroy the flavor conservation rule.

The recent progress in fabricating highly tunable TQDs aims to provide a platform for testing a variety of predicted novel quantum information processing functionalities and many-body effects. The goal of this work is to analyse the transport and thermodynamic properties of the SU(3) Kondo effect in highly symmetric capacitively-coupled TQD. Similar study has very recently been performed in Ref. [51], where comparison can be made, our results agree with theirs. We also study the effect of local perturbations on the SU(3) singlet Kondo state such as asymmetrical lead-dot couplings, finite interdot tunneling rates, non-equal charging energies, etc. Generally, these perturbations destroy the SU(3) singlet Kondo state, however, we propose a way to restore the Kondo resonance by properly gating the dot levels.

In order to investigate in a general framework the different regimes encountered for the the TQD system we consider the operators of the SU(3) Lie algebra which describe the orbital (flavor) degree of freedom of the electrons. The thermodynamics analysis is performed by calculating the impurity orbital (flavor) susceptibility $\chi_{\text{imp}}(T)$, and the impurity entropy $S_{\text{imp}}(T)$. Our results indicate that SU(3) Kondo physics occurs when the QDs are tuned to single occupancy, $n = 1$, or double occupancy, $n = 2$, which is achieved away from the particle-hole symmetric point, contrary to what happens in the more familiar SU(2) and SU(4) Kondo cases where at half filling the Kondo effect is present. Consequently, the Kondo peak itself is not symmetric with respect to the chemical potential as visible in the spectral densities for each dot. These values of the occupancy have important consequences for the linear conductance. In accordance with the Friedel-Langreth sum rule, the linear conductance is $G = G_0 \sin^2 \delta$ where the scattering phase shift $\delta$ is approximately given by $\delta = \pi n/N$; here $n = \langle \hat{n} \rangle$ is the total TQD occupation and $N = 3$, while $G_0$ is defined as $G_0 = e^2/h$ (note that we are considering a spinless system, thus the spin factor 2 is not present in $G_0$).

Therefore, in the SU(3) Kondo regime with $n = 1$ and $n = 2$ one has

$$G_{\text{Kondo}} = \frac{3}{4} e^2/h .$$

(1)

This result must be compared to that at the p-h symmetric point where $\delta = \pi/2$, and thus

$$G_{p-h} = e^2/h .$$

(2)

This paper is organized as follows. In Sec. I we introduce the model Hamiltonian to describe the TQD setup and discuss the theoretical tools to solve it. Section II is devoted to the study of the emergence of the SU(3) Kondo regime as a function of various parameters, namely the dot level position ($\epsilon_i$), the interdot Coulomb interaction ($V_i$), and the lead-dot tunneling couplings ($\Gamma_i$). The discussion is based on the thermodynamics and we investigate the behavior of the impurity orbital susceptibility $\chi_{\text{imp}}(T)$ and the impurity entropy $S_{\text{imp}}(T)$. In Sec. III we list some signatures of the SU(3) Kondo state in the transport measurements. In Sec. IV we study the robustness of the SU(3) orbital Kondo singlet against diverse perturbations, namely, asymmetric lead-dot tunneling couplings, different on-site energy values and possible leaking effects described by nonzero inter-dot tunneling rates. In Sec. V we briefly consider the generalization to the spinfull problem and discuss the different kinds of the Kondo effect expected in that case. Finally our main conclusions are summarized in Sec. VI.

II. MODEL AND METHODS

Figure 1: (Color online) Schematic representation of the capacitively coupled triple quantum dot system. Each quantum dot is attached to two electron reservoirs. We assume that a sufficiently large external magnetic field is applied to fully polarize the electrons, so that we may consider the system to be spinless. The only interaction between each pair of quantum dots is purely capacitive. Inter-dot charging energies (denoted by $V$) are assumed to be the same: they are characterized by the capacitance $C$, $V = e^2/2C$. Dashed lines indicate the electron transport through each dot.

We model the TQD system (see Fig. 1) using a Hamiltonian consisting of three copies of the non-interacting resonant-level
model (each describing one QD and the effective single channel of the electrons that the dot hybridizes with) and a coupling term which includes the inter-dot interactions and any possible inter-dot tunneling:

$$H = \sum_{i=1}^{3} H_i + H_{\text{int}},$$  \hspace{1cm} (3)

with

$$H_i = \sum_{k} \epsilon_k c_{k,i}^\dagger c_{k,i} + \epsilon_i d_i^\dagger d_i + v_i \sum_{k} \left( c_{k,i}^\dagger d_i + \text{h.c.} \right),$$  \hspace{1cm} (4)

and

$$H_{\text{int}} = \sum_{\langle i,j \rangle} \left[ V_{ij} n_i n_j + t_{ij} \left( d_i^\dagger d_j + \text{h.c.} \right) \right].$$  \hspace{1cm} (5)

Here $c_{k,i}^\dagger$ is the creation operator for an electron with momentum $k$ in channel $i$, while $d_i^\dagger$ is the creation operator for an electron in dot $i$; the occupancy operator is defined as $n_i = d_i^\dagger d_i$. Assuming flat conduction bands, the hybridisation of each channel to the attached dot is characterized by a single number, $\Gamma_i = \pi \rho \nu_i^2$, where $\rho$ is the density of states in the band which we take to be constant and of width $2D$ (flat-band approximation). Hereafter, we consider all energies in units of the half-bandwidth, $D = 1$. $V_{ij}$ is the charge repulsion between two dots, while $t_{ij}$ is the hopping amplitude between two dots. For symmetrical configurations we simplify the notation as $\epsilon \equiv \epsilon_i$, $\nu \equiv \nu_{ij}$. Notice that this model is similar to the Coqblin-Schrieffer SU($N$) model.

The Coqblin-Schrieffer model describes an impurity in the $N = 2j + 1$ representation of the SU($N$) total angular momentum group. The equivalence is established on low-temperature scales where the charge fluctuations are quenched. Assuming that the conduction bands are particle-hole (p-h) symmetric ($\epsilon_{-k} = -\epsilon_k$), the p-h transformation ($d_i^\dagger \rightarrow d_i$, $c_k^\dagger \rightarrow c_{-k}$, $c_k \rightarrow c_{-k}$, etc.) leads to (up to irrelevant constants)

$$\hat{H}_i = \sum_k \epsilon_k c_{k,i}^\dagger c_{k,i} + (-\epsilon_k) d_i^\dagger d_i + (-v_i) \sum_k \left( c_{k,i}^\dagger d_i + \text{h.c.} \right),$$  \hspace{1cm} (6)

and

$$\hat{H}_{\text{int}} = \sum_{\langle i,j \rangle} \left[ V_{ij} (1 - n_i)(1 - n_j) - t_{ij} \left( d_i^\dagger d_j + \text{h.c.} \right) \right].$$  \hspace{1cm} (7)

Therefore

$$\tilde{\epsilon}_i = -\epsilon - \sum_{\langle i,j \rangle} V_{ij},$$  \hspace{1cm} (8)

The model is p-h symmetric only for $t_{ij} = 0$, since finite inter-dot hopping breaks the bipartiteness. (The sign change of the hybridization $v_i$ is of no physical consequence.) For a symmetric configuration, the model is p-h symmetric around the point $\epsilon = -V$. Therefore the parameter $\delta = \epsilon + V$ is a measure of the departure from the p-h symmetry. It must be emphasized that the SU(3) Kondo effects that are discussed in the following occur away from the p-h symmetric point where the impurity charge fluctuates. This implies that the Kondo peak itself is not symmetric (confirmed by numerics, see below).

The standard (Gell-Mann) parametrisation for the generators of the SU(3) Lie algebra is $K_\lambda = \lambda_\alpha/2$ with $\lambda_\alpha$ being Gell-Mann matrices:

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$\lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

$$\lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ i & 0 & 0 \end{pmatrix}, \quad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}. $$  \hspace{1cm} (9)

We thus define the SU(3) operators for the TQD system as

$$O_a^{\text{imp}} = \sum_{ij} c_{k,i}^\dagger (K_a)_{ij} c_{k,j},$$

$$O_a^{\text{total}} = O_a^{\text{imp}} + \sum_k O_a^{(k)},$$

where $a = 1, \ldots, 8$, while $i$ and $j$ range over the three channels, and $k$ ranges over all conduction-band momenta. The Casimir operator of SU(3) is defined as

$$K_{\text{total}}^2 = \sum_{a=1}^{8} (O_a^{\text{total}})^2. $$  \hspace{1cm} (11)

In a fully SU(3) symmetric case, the traces $\text{Tr}(O_a^2)$ are all equivalent. In numerical calculations, it is thus sufficient to calculate the expectation value of a single $O_a^{\text{imp}}$ operator; the most convenient choice is $O_3^{\text{imp}}$. The expectation value of $\langle K_{\text{total}}^2 \rangle$ is then 8 times this value.

The behavior of an impurity system can be analyzed by studying its thermodynamic properties. In the following section we will consider the impurity orbital susceptibility $\chi_{\text{imp}}(T)$ and the impurity entropy $S_{\text{imp}}(T)$. These two quantities serve to establish the range of parameters for which the SU(3) spin Kondo physics is encountered. In the fundamental representation of SU(3) one has $\langle K^2 \rangle = 4/3$. In the high-temperature regime where all eight dot states are equally probable, one has $\langle K^2 \rangle = (6 \times 4/3 + 2 \times 0)/8 = 1$, since there are six singly occupied states (by either one electron or by one hole) and two states corresponding to totally empty and totally full system. The impurity SU(3) orbital susceptibility (more precisely, this is the impurity contribution to the total system orbital susceptibility) is defined as

$$\chi_{\text{imp}}(T) = \beta \left( \langle K_{\text{total}}^2 \rangle(T) - \langle K_{\text{total}}^2 \rangle_0(T) \right), $$  \hspace{1cm} (12)
where the bracket with subscript 0 denotes the result for the system without the dots (i.e., the Hamiltonian $H$ consists only of the conduction bands). Here $\beta = 1/k_B T$ with $k_B$ the Boltzmann constant. The value of $k_B T \chi(T)$ therefore indicates the presence of a finite effective orbital local moment on the TQD and it can be used to classify the fixed points.\textsuperscript{55,56}

The impurity entropy is a measure of the number of the effective degrees of freedom of the TQD at a given parameter configuration. It is defined through

$$S_{\text{imp}}(T) = \frac{(E - F)}{T} - \frac{(E - F)_0}{T},$$

(13)

where $E = \langle H \rangle = T\text{Tr}[H \exp(-H/k_B T)]$ and $F = -k_B T \ln \text{Tr}[\exp(-H/k_B T)]$.

We also compute the dot spectral functions $A(\omega; T)$ and compute the differential conductance through each dot using the Meir-Wingreen formula as implemented in the “NRG Ljubljana” code. We have used the discretization parameter $\Lambda = 8$ with the $z$-averaging over $N_z = 8$ values. We have verified that such a large value of $\Lambda$ still produces reliable results by performing a convergence study as a function of $\Lambda$ down to $\Lambda = 2$. In the NRG truncation, we have kept states with energy up to $10\omega_N$ where $\omega_N$ is the characteristic energy scale at the $N$-th NRG step, or at most 6000 states. For calculating the spectral functions, we have used the complete Fock space method.\textsuperscript{56,57,58,59} Very recently, a study of the fully symmet-ric SU(3) model has been performed with an implementation of the NRG which can explicitly use the SU(3) symmetry of the model to simplify the calculations.\textsuperscript{57} Here we only use the U(1) total-charge-conservation symmetry, thus the calculations are significantly more time-demanding. However, our approach makes it possible to study the effects of the symmetry breaking terms, which is important for physical realizations of this model.

III. NUMERICAL RESULTS: VALENCE FLUCTUATING AND THE SU(3) KONDO REGIMES

In order to identify the different regimes of the TQD system we consider the thermodynamic and transport properties. In Fig.\textsuperscript{2} we show the basic results for the fully SU(3) symmetric case where all the dots and hybridizations are equivalent. The lead-dot couplings have common value of $\Gamma = 0.01$, and there is no inter-channel tunneling (i.e., $t \equiv 0$). Since the system is symmetric with respect to the point $\epsilon = -V$ for this choice of parameters, we consider only the value of the on-site energy $\epsilon$ below $-V$ (i.e., $\delta < 0$); other results can be obtained by an appropriate p-h transformation.

We observe that for a range of on-site energies $-0.35 \lesssim \epsilon \lesssim -0.25$, the occupancy reaches values close to 2. In this case, the system evolves from the free-orbital fixed point (fp) with impurity entropy of 3 ln 2 to a local-moment fp with triple degeneracy (indicated by a ln 3 plateau in the impurity entropy) as the temperature decreases below the charge-fluctuation scale of $V$. The triple degeneracy is finally lifted at low temperatures and then we reach a non-degenerate strong-coupling fp corresponding to the SU(3) Kondo regime. In this regime the zero-temperature linear conductance is near 3/4, as predicted in Ref.\textsuperscript{59} based on the Friedel sum rule arguments [see Eq. (1)].

A very different behavior is found near the p-h symmetric point at $\epsilon = -V$. Here the system evolves from the free-orbital to the valence-fluctuation fp with entropy ln 6 (only visible as a weak bulge in the $S_{\text{imp}}(T)$ curve in Fig.\textsuperscript{2}). In this case the valence-fluctuation regime corresponds to charge fluctuations from $n = 1$ to $n = 2$ charge states. The entropy is eventually reduced from ln 6 to zero at some low temperature. In this case the entropy is released as the system evolves to the strong-coupling fp without passing through the local-moment fp.

By reducing the dot-lead hybridisation by half, i.e., for $\Gamma =
0.005, as shown in Fig. 3, the SU(3) Kondo regime is even more clearly discernible and we can see that the occupancy is pinned to the value 2 for a much broader range of dot potential energies. Here, the conductance reaches the universal value of $G = 3/4(2e^2/h)$ for a wide range of $\epsilon$ due to a much more robust SU(3) Kondo state.

In the SU(3) Kondo regime, the dot spectral density, shown in Fig. 4 displays a Kondo resonance with a maximum height shifted away from the Fermi level. As previously noticed this is the result of having the SU(3) Kondo regime away from the $p$-$h$ symmetric point. In addition, the shifted spectral density produces a zero-temperature linear conductance $G = 3/4(e^2/h)$, which is by itself a hallmark of the occurrence of the SU(3) Kondo physics. This is in contrast with the SU(4) case where the linear conductance coincides in value with the linear conductance for the SU(2) Kondo effect.

The thermodynamic properties of the SU(3) Kondo regime are studied in more detail in Fig. 5. In order to gain some intuition about the role of the Kondo correlations in the SU(3) orbital susceptibility we compare the case of an uncoupled TQD system, where all three lead-dot hybridizations are $\Gamma = 0$, with the case where the TQD is connected to leads and the

Figure 3: (Color online) Temperature dependence of the impurity entropy (left panels) and the zero-temperature dot spectral function (right panels) for a range of the on-site energies $\epsilon$. Same parameters as in Fig. 2 but with smaller hybridization, $\Gamma = 0.005$. We plot the positive-frequency side of the spectral function on the logarithmic frequency scale. The dashed line corresponds to the characteristic conduction of $G = (3/4)(e^2/h)$.

Figure 4: (Color online) Spectral function in the SU(3) Kondo regime. The triple quantum dot system is symmetric and the total occupancy is $\langle n \rangle = 2$. Note the pinning of the zero-frequency spectral density to the value $A(0) = (3/4)/\pi \Gamma$ and the important fact that the actual Kondo peak is displaced away from $\omega = 0$.

Figure 5: (Color online) Thermodynamic properties in the SU(3) Kondo regime. We consider a symmetric TQD system. The total occupancy of the triple quantum dot, $\langle n \rangle = 2$. We compare the cases of a decoupled triple quantum dot system ($\Gamma = 0$) and the triple quantum dot connected to the leads ($\Gamma = 0.005$) in which the Kondo correlations are present.
SU(3) Kondo state builds up. In the high-temperature limit, in both cases the spin susceptibility is 1 and all 8 TQD states are equally probable, thus there is \(\ln 8 = 3\ln 2\) impurity entropy. As the temperature decreases below \(V\), so that the charge fluctuations are frozen out, the SU(3) susceptibility of \(4/3\) is established, as expected for the fundamental triplet representation of SU(3). This is the local-moment fp. The decoupled system stays in this fixed point down to \(T = 0\), while at finite \(\Gamma\) the local moment is screened in the SU(3) Kondo effect and the susceptibility vanishes, as expected. At this point the system is in the non-degenerate strong-coupling fp in which the ground state corresponds to a SU(3) Kondo singlet state. Notice that the transition from the free-orbital to the local-moment regime and then eventually to the strong-coupling regime is fully analogous to the behaviour in the standard single-impurity Anderson model with the SU(2) symmetry.\(^{55,56,58}\) We also emphasize that the low-temperature parts of the impurity susceptibility and impurity entropy are universal and that the scaling of the results for different parameters is observed if the temperature axis is rescaled by an appropriately defined Kondo temperature \(T_K\) (see below).

For completeness we also analyse the p-h symmetric point, in which the only low-temperature scale is \(\Gamma\) itself and there is no Kondo-like screening. In this model, the p-h symmetric point corresponds to a valence-fluctuation regime where charge fluctuations occur. In Fig. 6 the temperature dependence of the entropy is shown for a symmetric TQD and various \(\Gamma\) values when \(\epsilon = -V\). At high temperatures the TQD is found in the free-orbital regime where the TQD entropy is \(\ln 8\). Then, the system crosses over on the temperature scale of \(V\) to a valence-fluctuation fp with a six-fold degenerate ground state in which the entropy reaches the value of \(\ln 6\). In this case, there can be either a single electron or a single hole in the three dots for a total of six states with the same energy. Decreasing further the temperature the system crosses over to the non-degenerate ground state with zero entropy at the temperature scale of \(\Gamma\), see Fig. 6. There is no further dynamically generated low-energy scale in this case.

The zero-temperature fixed points for different \(\epsilon\) form a line of fixed points which are related by the different strength of the residual potential scattering experienced by the quasiparticles. For an overview of the system behavior, in Fig. 7 we plot the zero-temperature total TQD occupancy, linear conductance, and charge fluctuations as a function of the on-site energy \(\epsilon\) for several choices of the hybridization \(\Gamma\). The emergence of the Kondo plateau for low enough \(\Gamma\) is clearly visible; it coincides with the regions of low charge fluctuations in the TQD.

### IV. EVIDENCE OF SU(3) KONDO CORRELATIONS IN TRANSPORT MEASUREMENTS

In the previous section, we have demonstrated the occurrence of the SU(3) Kondo effect by considering the thermodynamic properties. Usually, one way to probe the existence of Kondo correlations in QD systems is to measure the exponential dependence of the Kondo energy scale \(k_B T_K\) with the inverse hybridization \(1/\Gamma\) as

\[
\ln T_K \propto -\frac{1}{\Gamma}. \tag{15}
\]

In the NRG calculations this dependence is demonstrated by using a \(T_K\) defined from the entropy curve as \(S_{\text{imp}}(T_K) = \ln 8 = 3\ln 2\).
hybridisation parameters \( \Gamma \) we uncover the exponential dependence, see the lower panel of Fig. 8.

\[
G(T) = G_0 \left(1 + (2^{1/s} - 1)(T/T_K)^2\right)^{-s},
\]

with \( s = 0.23 \) for the SU(2) case and with \( s = 0.28 \) for the SU(3) Kondo case. The value of \( s = 0.28 \) has been extracted from the NRG results for \( G(T) \). The fitting to \( G(T) \) is performed for a symmetric TQD at \( \epsilon = -0.2 \), and \( \Gamma = 0.005 \), see Fig. 9. It is interesting to notice that a single fit formula, Eq. (15), applies over many orders of magnitude in temperature in a number of quantum impurity models that exhibit Kondo effects of very different kinds; see, for example, Refs. [62,63].

Since the spectral function \( A(\omega) \) is asymmetric, care is needed in extracting the width of the spectral function peak from the differential conductance measurements at finite bias voltage (even when the non-equilibrium effects are neglected). When properly done, by measuring \( T_K \) and then varying \( \Gamma \) one should be able to get a relation that matches Eq. (15).

Another signature of the SU(3) Kondo physics could be detected through the temperature dependence of the linear conductance \( G \). Close to zero temperature, \( G \) is \( 3/4 \) in units of the conductance quantum \( G_0 = e^2/h \) (note the absence of factor 2 in this spinless case). At small but finite temperatures, we find that the low-temperature conductance fits, similarly to the SU(2) Kondo case, to the empirical formula of the general form

\[
G(T) = G_0(1 + (2^{1/s} - 1)(T/T_K)^2)^{-s},
\]

In view of this result, the occurrence of SU(3) Kondo correlations in a TQD experiment could be demonstrated by performing transport measurements, for instance by measuring the Kondo temperature \( T_K \). Usually this is achieved by identifying the half width at the half maximum (HWHM) of the non-linear conductance peak through one of the dots with \( T_K \). This measurement would, however, be rendered problematic in this system due to the asymmetric shape of the Kondo resonance. In \( dI/dV \) measurement with finite bias, the current is namely given approximately by

\[
I(T, V) = \int [f_L(\omega) - f_R(\omega)] \pi \Gamma A(\omega, T)d\omega,
\]

where we have neglected the voltage-dependence of the spectral function, and we assume \( f_L(\omega) = f(\omega - V/2) \) and \( f_R = f(\omega + V/2) \). In the zero-temperature limit, we thus find approximately

\[
\frac{dI}{dV} = G_0 \pi \Gamma \frac{A(V/2, 0) + A(-V/2, 0)}{2}.
\]
noteworthy that the Kondo spectral peaks are better visible in the close-up shown as an inset in Fig. 11. It is spectral functions show \( \Gamma \) case of asymmetrical lead-dot coupling configuration where dots 2 and 3 are becomes decoupled and it is only weakly conducting. A high value (approaching, in fact, the unitary limit), while that for \( \Gamma_2 \) is strongly suppressed. This is related to the fact that for \( \Gamma_3 \) is different. The same happens when all three \( \Gamma_i \) are different.

As already mentioned, the asymmetry of the lead-dot couplings in the SU(3) Kondo effect is analogous to the SU(2) Kondo physics in the presence of ferromagnetic contacts. In the latter case, the Kondo resonance is split due to the appearance of an induced exchange field because of the polarized contacts. The same physical behavior is obtained for the SU(3) Kondo case. Figure 11 shows this result. We plot the spectral densities for the dot 1 and dot 2, denoted as \( A_1(\omega) \) and \( A_2(\omega) \). We consider the case of symmetric couplings \( \Gamma = \Gamma_1 = \Gamma_2 = \Gamma_3 \) in which \( A_1(\omega) = A_2(\omega) \) and the case of asymmetrical lead-dot coupling configuration where \( \Gamma_2 = \Gamma_3 = 0.005 \) and \( \Gamma_1 = 0.003 \). In the latter case the two spectral functions show SU(3) Kondo-peak splitting which is better visible in the close-up shown as an inset in Fig. 11. It is noteworthy that the Kondo spectral peaks for \( A_2 = A_3 \) reach a high value (approaching, in fact, the unitary limit), while that for \( A_1 \) is strongly suppressed. This is related to the fact that the dots 2 and 3 are SU(2) Kondo screened, thus their zero-bias conductance remains nearly unitary, while the dot 1 becomes decoupled and it is only weakly conducting.

### B. Unequal on-site dot energies

The SU(3) Kondo state can also be destroyed by having non-equal dot level energies. This case is illustrated in Fig. 12.
where it is shown how the SU(3) symmetry is broken by changing the on-site energy $\epsilon_1$ away from the common value $\epsilon$, i.e., $\epsilon_2 = \epsilon_3 = \epsilon + \delta \epsilon_1$, with $\delta \epsilon_1$ being the detuning. The resulting new state depends on the direction of the detuning. For positive detuning $\delta \epsilon_1 > 0$, shown in the upper panel in Fig. 12, the SU(3) Kondo effect is quenched on the energy scale of the detuning. However, for negative detuning $\delta \epsilon_1 < 0$, shown in the lower panel, the system evolves from the three fold degenerate local moment $f_p$ with $S_{imp} = \ln 3$ to a two fold degenerate local moment $f_p$ in which $S_{imp} = \ln 2$. In this case the SU(2) local moment emerges from two states that originally formed the SU(3) triplet local moment.

Figure 12: (Color online) Temperature dependence of the impurity entropy for a range of the parameter $\delta \epsilon_1$ defined as $\epsilon_2 = \epsilon_3 = \epsilon + \delta \epsilon_1$, while $\epsilon_2 = \epsilon_3 = \epsilon$ with $\epsilon = -0.3$. The rest of the parameters correspond to a symmetric triple quantum dot configuration with $V = 0.2$, $\Gamma = 0.005$.

C. Finite interdot tunneling: $t \neq 0$

We have also investigated the fact that the three-fold symmetry can also be broken by a finite interdot tunneling. The behavior yet again depends on the sign of $t$: the ground state may either be a single state (not Kondo screened) or a two-fold degenerate pair which is Kondo screened. The positive $t$ case is considered in the upper panel of Fig. 13. Here the entropy evolves from $\ln 3$ to zero on the temperature scale of $t$ signaling the destruction of the SU(3) Kondo singlet. For negative $t$, the lower panel in the figure shows that the impurity entropy evolves from $\ln 3$ to $\ln 2$ on the temperature scale of $|t|$ and the latter corresponds to local moment $fp$ of two-fold pair of states and it constitutes a SU(2) local-moment which undergoes the SU(2) Kondo screening at much lower temperatures.

D. Restoration of the SU(3) Kondo physics

Symmetry can also be broken by having different inter-dot charge repulsion parameters $V_{ij}$. In experiments, the capacitive couplings $V_{ij}$ are the most difficult to control, followed by the inter-dot hopping parameters $t_{ij}$ and hybridizations $\Gamma_i$, while the on-site energies $\epsilon_i$ are typically the easiest to tune. There are eight “directions” for an SU(3) symmetry-breaking field, corresponding to the eight generators of this symmetry. A consideration of the Gell-Mann matrices in Eq. (9) suggest that two ($\lambda_3$ and $\lambda_8$) are associated with the energy levels, since they are diagonal, while the remaining six are out-of-diagonal and thus associated with the inter-dot tunneling. This immediately suggests that symmetry breaking by tunneling cannot be compensated electrostatically. It is thus essential, first of all, to ensure that the inter-dot tunneling is low-enough for the observation of the SU(3) Kondo effect. In essence, the tunneling rate should be much smaller than the anticipated Kondo temperature scale (in appropriate frequency units). Any remaining asymmetry then corresponds to SU(3) “fields” in $\lambda_3$ and $\lambda_8$ directions which arise from
asymmetric $\epsilon_i, \Gamma_i$ and $V_{ij}$. Assuming that the three on-site energies $\epsilon_i$ can be freely and independently tuned, it appears possible to compensate the asymmetries in $\Gamma_i$ and $V_{ij}$ since there are three parameters to drive two “fields” to zero. We demonstrate this procedure in Fig. 14 where an asymmetry in the hybridization constants is compensated by tuning the on-site potentials. Thus, making use of the high degree of tunability in QD devices, any source of symmetry breaking which naturally arise from the manufacturing process can be compensated by properly adjusting the gate voltages.

![Figure 14](Color online) Restoration of the SU(3) Kondo effect in an asymmetrically lead-dot coupled triple quantum dot ($\Gamma_1 = 0.004$, and $\Gamma_2 = \Gamma_3 = 0.005$) by tuning the on-site dot potential $\epsilon_i = \epsilon + \delta \epsilon_i$, with $V = 0.2$, and $\epsilon = -0.3$. The SU(3) symmetry is effectively restored for $\delta \epsilon_i = 3.25 \times 10^{-5}$, which is indicated by the impurity curve having the universal SU(3) shape. The curves for parameters near the restoration point show some wiggles; these are numerical artifacts.

VI. SPINFULL TRIPLE QUANTUM DOT

For completeness, in this section we briefly discuss the version of our model with spin degrees of freedom and additional on-site electron-electron repulsion terms $U$. The Hamiltonian takes the form of three copies of the single-impurity Anderson model and a coupling term with all inter-dot terms:

$$H = \sum_{i=1}^{3} H_i + H_{\text{int}}, \quad (19)$$

where

$$H_i = \sum_{k,\sigma} \epsilon_k c_{k,\sigma,i}^\dagger c_{k,\sigma,i} + \epsilon_i n_i + U_i n_{i\uparrow} n_{i\downarrow} + v_i \sum_{k,\sigma} \left( c_{k,\sigma,i}^\dagger d_{\sigma,i} + \text{h.c.} \right), \quad (20)$$

and

$$H_{\text{int}} = \sum_{\langle i,j \rangle} V_{ij} n_i n_j + t_{ij} \sum_{\sigma} \left( d_{\sigma,i}^\dagger d_{\sigma,j} + \text{h.c.} \right). \quad (21)$$

Most terms have the same meaning as in the spinless model, Eq. (5), but now $n_{\sigma,i} = d_{\sigma,i}^\dagger d_{\sigma,i}$ and $n_i = n_{\uparrow,i} + n_{\downarrow,i}$.

Here we will only consider some features of this model. We restrict our attention to a model with no inter-dot tunneling, $t_{ij} = 0$, and full orbital symmetry, i.e., $\epsilon_i = \epsilon, U_i = U$, $V_{ij} = V$, and $v_i = v$ (or, equivalently, $\Gamma_i = \Gamma$). Despite the high symmetry of this problem, it is still too complex for a detailed study using the NRG technique. For this reason, we resort to a different numerical approach, the Gunnarson-Schönhammer variational method. Following Refs. [44 and 65] we form a variational ansatz for the ground state wavefunction $|\bar{0}\rangle$ of the Hamiltonian (19).

$$|\bar{0}\rangle = \sum_{n_1 n_2 n_3} \lambda_{n_1 n_2 n_3} P_{n_1 n_2 n_3} |\bar{0}\rangle + \sum_{k,i,n_1 n_2 n_3} \lambda_{k,i,n_1 n_2 n_3} \sum_{\sigma} d_{k,\sigma,i}^\dagger c_{k,\sigma,i} |\bar{0}\rangle + \sum_{k,i,n_1 n_2 n_3} \lambda_{k,i,n_1 n_2 n_3} \sum_{\sigma} n_{\sigma,i} |\bar{0}\rangle. \quad (22)$$

Here $|\bar{0}\rangle$ is the ground state wavefunction of the noninteracting part ($U = V = 0$) of the Hamiltonian (19) with renormalized dot energy levels $\tilde{\epsilon}$ and lead-dot couplings $\tilde{v}$.

$$\tilde{H}(\tilde{\epsilon}, \tilde{v}) = \sum_{k,\sigma,i} \epsilon_{k,\sigma,i} c_{k,\sigma,i}^\dagger c_{k,\sigma,i} + \sum_{i} \tilde{\epsilon} n_i + \sum_{k,\sigma,i} \left( \tilde{v} d_{\sigma,i}^\dagger c_{k,\sigma,i} + \text{h.c.} \right). \quad (23)$$

Projectors $P_{n_1 n_2 n_3}$ project this state to subspaces with $n_i = 0, 1, 2$ electrons in the $i$-th dot. Variational terms in the second and the third row of Eq. (22) provide states containing an electron above the Fermi energy and a hole below the Fermi energy in one of the leads, respectively. An approximation to the true Hamiltonian (19) ground state energy $E_0(\tilde{\epsilon}, \tilde{v})$ and the corresponding ground state wavefunction coefficients $\lambda_{n_1 n_2 n_3}$ are calculated by solving the Schrödinger equation within the Hilbert space of the ansatz. The ground state energy is then further minimized with respect to $\tilde{\epsilon} \to \bar{\epsilon}_0$ and $\tilde{v} \to \bar{\epsilon}_0$, providing us with the noninteracting part of the Fermi liquid quasiparticle Hamiltonian $\tilde{H}(\bar{\epsilon}_0, \bar{\epsilon}_0)$ of our problem which we use to calculate the zero temperature conductance. The occupancy of the dots and its fluctuations are calculated from the ground state wavefunction $|\bar{0}\rangle$.

To study the interplay of the inter-site and on-site charge repulsion terms $U$ and $V$, we first fix $U$ and increase $V$. For $V = 0$, the system consists simply of three copies of the single-impurity Anderson model, the properties of which are well known. In the interval $-U + \Gamma \lesssim \epsilon \lesssim -\Gamma$, we expect the emergence of the SU(2) Kondo effect in each of the three channels independently, thus a plateau of unitary conductance through each dot (note that the unitary limit is now $2e^2/h$ due to the spin factor). For non-zero but moderate $V < U$, we expect the occurrence of collective Kondo screening which affects all three quantum dots. In this case, in addition to the spin degree of freedom on each dot, there is an orbital degree of freedom, as in the spinless case that
has been discussed in the previous sections. The two degrees of freedom may become intertwined like in the SU(4) Kondo effect in carbon nanotubes where the spin and isospin degrees of freedom are combined. Here, however, the symmetry is SU(2)\textsubscript{spin} × SU(3)\textsubscript{orbital} and richer behavior is expected. This model is closely related to the impurity models studied in the context of dynamical mean-field theory for correlated bulk metals, in particular for transition-metal compounds where the three-fold degenerate \( t_{2g} \) d-electron orbitals play the main role. The results in Fig. 15 indicate the emergence of three different kinds of the Kondo plateau for on-site energies corresponding to the total TQD occupancy being pinned to an integer value. At the p-h symmetric point, we observe a Kondo plateau for all values of \( V \leq U \); this is thus contrary to the behavior found in the spinless model where in this regimes the valence fluctuates and the Kondo effect does not occur. Two additional types of the Kondo effect are present, one for single-electron (single-hole) occupancy, \( \langle n \rangle = 1, 5 \), characterized by the conductance pinned to \( G = 2e^2/h \sin^2[(\pi/2)(1/3)] = 0.5(e^2/h) \), another for two-electron (two-hole) occupancy, \( \langle n \rangle = 2, 4 \), characterized by \( G = 2e^2/h \sin^2[(\pi/2)(2/3)] = 1.5(e^2/h) \). In the first case, the single electron has both spin and orbital degree of freedom (both in the fundamental SU(2) and SU(3) representations), thus this corresponds to the SU(6) Kondo effect. In the second case, two electrons are combined into a more complex object which is then Kondo screened.

VII. CONCLUSIONS

We have demonstrated the formation of the SU(3) singlet Kondo state in a spinless triple quantum dot system. We have performed a thermodynamics analysis with the help of the magnetic susceptibility (\( \chi_{\text{imp}} \)) and the impurity entropy (\( S_{\text{imp}} \)). For a highly symmetric triple quantum dot we find, when the dot system charge is either \( n = 2 \) or \( n = 1 \) (away from the particle-hole symmetric point for which \( n = 1.5 \)), that the system evolves from the free-orbital regime at high temperatures with \( T\chi_{\text{imp}} = 1 \) and \( S_{\text{imp}} = \ln 8 \) to the three-fold degenerate local moment fixed point with \( T\chi_{\text{imp}} = 4/3 \) and \( S_{\text{imp}} = \ln 3 \) towards a non-degenerate strong coupling fixed point where the SU(3) spin is totally screened. This cross-over occurs on an exponentially low temperature scale, \( \ln T_K \propto -1/\Gamma \). In contrast, for the electron-hole symmetric point, the system evolves from the free-local moment regime to a valence-fluctuating fixed point where the entropy \( S_{\text{imp}} = \ln 6 \), and then to zero on the scale of \( \Gamma \). Additionally, we have investigated possible perturbations that affect the formation of the SU(3) singlet Kondo state in real setups. Among these perturbations we have studied how non-symmetrical lead-dot couplings or on-site potential energies, and finite inter-dot tunneling rates break the SU(3) Kondo physics. We have described the procedure to restore the SU(3) Kondo physics in real systems by properly tuning the on-site dot energies. Finally, we described the more complex behavior of the spinfull case where the Kondo effect occurs for all integer occupancies of the triple quantum dot, including at the particle-hole symmetric point.

Figure 15: (Color online) Occupancy \( n \), differential conductance \( G \) and charge fluctuations \( \delta n^2 = \langle n^2 \rangle - \langle n \rangle^2 \) as a function of the on-site energy \( \epsilon = -U/2 - 2V + \delta \) for on-site repulsion \( U = 0.32 \) and for a range of interdot repulsions \( V \). \( \Gamma = 0.01 \).

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