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Kondo temperature of SU(4) symmetric quantum dots

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A path integral approach is used to derive a closed analytical expression for the Kondo temperature of the SU(4) symmetrical Anderson model. In contrast to the SU(2) case, the prefactor of the Kondo temperature is found to display a peculiar orbital-energy (gate voltage) dependence, reflecting the presence of various SU(4) mixed valence fixed points. Our analytical expressions are tested against and confirmed by numerical renormalization group computations.

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Introduction. Much of our perception of strongly interacting fermion systems such as heavy fermions [1], molecules and quantum dots attached to electrodes [2], correlated states of interacting cold atoms [3], or phenomena such as the Mott transition [4] relies on the detailed study of magnetic impurities and the Kondo effect. The latter consists of the dynamical screening of a local spin entity, interacting antiferromagnetically with surrounding itinerant electrons [5], and provides the simplest example of asymptotic freedom. The fundamental energy scale at which the Kondo screening develops is called the Kondo temperature $T_{\rm K}$. Our understanding of this curious effect has been strengthened by several recent experiments on quantum dot (QD) systems and nanotubes, which not only allow an accurate control of the model parameters, but also enable one to study out-of-equilibrium phenomena [2,6] and to realize exotic correlated states such as the two-channel Kondo state [7] or the SU(4) Kondo effect [6,8,9] in a controlled manner.

One of the most fascinating features of the Kondo effect is that of *universality*: apart from a few dimensionless numbers characterizing the asymmetry of the leads and electron-hole symmetry, at low temperatures or voltages, every physical quantity depends on the microscopic model parameters solely through $T_{\rm K}$. While determining $T_{\rm K}$ is therefore clearly of crucial importance, estimating it precisely is an utmost delicate problem. Its first estimate is due to Kondo [10], who constructed and studied a model of a local spin $\mathbf{S}$ (the spin on the QD or the molecule) coupled to the lead (conduction) electrons' spin density through an exchange coupling, $H_{\rm int} = J_0\, \mathbf{S}\cdot\mathbf{s}$. Kondo's exchange model contains, however, logarithmic singularities, which must be regularized by a bandwidth cutoff $\mathcal{D}_0$. The Kondo temperature is found to depend explicitly on this unknown parameter and is expressed as $T_{\rm K,SU(2)} \approx \mathcal{D}_0\sqrt{\nu_0 J_0}\exp[-1/(\nu_0 J_0)]$ for SU(2) spins [5], with ν_0 denoting the electrons' density of states. Unfortunately, $\mathcal{D}_0$ and J_0 being both somewhat arbitrary, the predictive power of this expression is limited.

A better estimate can be obtained through the analysis of Anderson's more elaborate impurity model [5], as first done by Haldane [11,12]. In Anderson's model, some local fermionic degrees of freedom d_τ of energy ε_d interact with each other by a local interaction of strength U and hybridize with the leads (conduction electrons) as described by the Hamiltonian

$$H_{\rm An} = \varepsilon_d \sum_\tau d_\tau^\dagger d_\tau + U \sum_{\tau<\tau'} n_\tau n_{\tau'} + t\sum_{k\tau}(c_{k\tau}^\dagger d_\tau + \text{H.c.}) + \sum_{k,\tau}\varepsilon_k c_{k\tau}^\dagger c_{k\tau}. \quad (1)$$

Here the operators $c_{k\tau}^\dagger$ create conduction electrons of energy ε_k and internal degree of freedom τ, which we call "spin" [13], and the strength of hybridization is characterized by the decay rate $\Delta = \pi\nu_0 t^2$. In contrast to the Kondo model, the Anderson model is *not* ultraviolet divergent and has a well-defined Kondo scale in terms of its three parameters, ε_d, U, and Δ, which Haldane determined accurately through a renormalization group analysis for the spin-$\frac{1}{2}$ case, $\tau = \uparrow,\downarrow$. A closer analysis of Haldane's work reveals, however, that to provide a precise estimate of the Kondo temperature, one also needs to account for charge (valence) fluctuations.

In this work, we study the SU(4) symmetrical Anderson model (with $\tau = 1,\ldots,4$) and determine its Kondo temperature (Fermi liquid scale) accurately. The study of the SU(4) case is motivated by its particular experimental relevance: signs of an emergent SU(4) symmetrical Kondo state were observed in carbon nanotubes [8] and vertical quantum dots [9], single-atom transistors [14], double-QD devices [6,15], and other exotic SU(4) Kondo regimes are also expected in fourfold-degenerate QD systems where both spin and orbital degrees of freedom are conserved in tunneling [15]. Here we develop a path integral formalism introduced in Ref. [16] (see also Ref. [17] for a similar approach) to show that, in contrast to the SU(2) case, the prefactor of the Kondo temperature has a curious dependence on the level position ε_d. This dependence is a fingerprint of the presence of various SU(4) mixed-valence fixed points, governing the charge transitions of the QD (d level). The right panel of Fig. 2 illustrates the importance of the prefactor in determining T_K by comparing it with the SU(2) constant prefactor. Our analytical predictions for $T_{\rm K}$ are found to agree quantitatively with numerical renormalization group (NRG) computations, which also confirm the presence and importance of SU(4) mixed-valence fixed points [18].

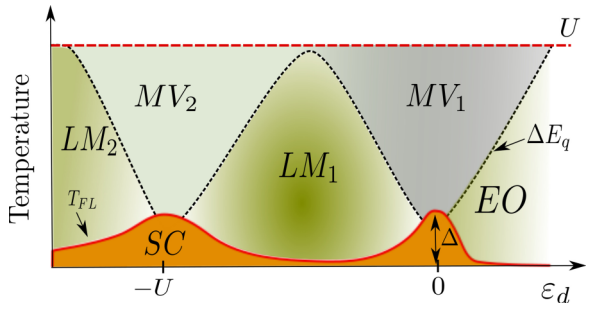

FIG. 1. (Color online) Sketch of the "phase diagram" of the SU(4) Kondo model. In the mixed-valence region MV_1 (MV_2) the fourfold-degenerate $q = 1$ state competes with the $q = 0$ empty orbital state (the sixfold-degenerate $q = 2$ state). In the local moment region LM_1 the $q = 1$ SU(4) spin produces Kondo effect and is screened below the Kondo scale, T_K, while in region LM_2 a sixfold-degenerate SU(4) spin is screened. EO and SC stand respectively for empty orbital and strong coupling [18].

The corresponding mixed-valence regions and the "phase diagram" of the SU(4) Kondo model are sketched in Fig. 1 [19]. In the mixed-valence regions MV_1 and MV_2 the fourfold-degenerate charge $q = 1$ state of the QD (d level) competes with the $q = 0$ empty orbital (EO) and the sixfold-degenerate $q = 2$ states, respectively. The SU(4) spins are formed at temperatures below the energy of the QD's charging excitations ΔE_q (in local-moment regions LM_1 and LM_2) and get screened at strong coupling (SC) below the Kondo scale T_K [18]. The scale ΔE_q vanishes, however, as one approaches the valence transition points, $\varepsilon_d \approx 0$ and $\varepsilon_d \approx -U$, where the mixed-valence fixed points determine the physics down to the Fermi liquid scale, $T_K \sim \Delta$. However, in the mixed-valence regime, there is no Kondo effect. Nevertheless there is still a crossover energy scale to a Fermi liquid regime and this energy scale is connected continuously to the Kondo temperature T_K.

To determine T_K, we focus on the Kondo regime of the QD, with $q = 1$, 2, and 3 electrons trapped on the fourfold-degenerate level, and establish a mapping between the SU(4) Anderson model and the SU(4) Kondo model [20], described by the exchange interaction, $H_{\rm exch}^{\rm SU(4)} = \frac{J}{2}\sum_{kk',\tau\tau'}(d_{\tau'}^\dagger d_\tau - 1/4)c_{k\tau}^\dagger c_{k'\tau'}$. We determine first J and the cutoff $\mathcal{D}$ by computing the logarithmic corrections to the amplitude of the exchange processes at energy ω,

$$\mathcal{J}(\omega) = J - \frac{N\nu_0}{2} J^2 \ln\frac{\omega}{\mathcal{D}} + \cdots, \tag{2}$$

in both models. Using then the well-known two-loop result for the Kondo temperature, $T_{K,\,SU(N)} = \mathcal{D}\sqrt[N]{N\nu_0 J/2}\exp[-2/(N\nu_0 J)]$, we obtain the Kondo temperature of the SU(4) Anderson model as

$$T_{K,SU(4)} = \mathcal{D}_{\rm eff}\sqrt[4]{2\nu_0 J_0}\, e^{-\frac{1}{2\nu_0 J_0}}, \tag{3}$$

$$\mathcal{D}_{\rm eff} = U\, f_q(\varepsilon_d/U), \tag{4}$$

with $J_0 = -2t^2U/[E_q(E_q+U)]$ the usual leading-order expression for the Kondo coupling, expressed in terms of the shifted energies $E_q = \varepsilon_d + (q-1)U$ [20].

Equation (3) differs from the SU(2) formula derived by Haldane in that the prefactor in Eq. (3) depends explicitly on the orbital energy (gate voltage) ε_d through the function f_q, specified later [21]. We emphasize that Eq. (3) incorporates

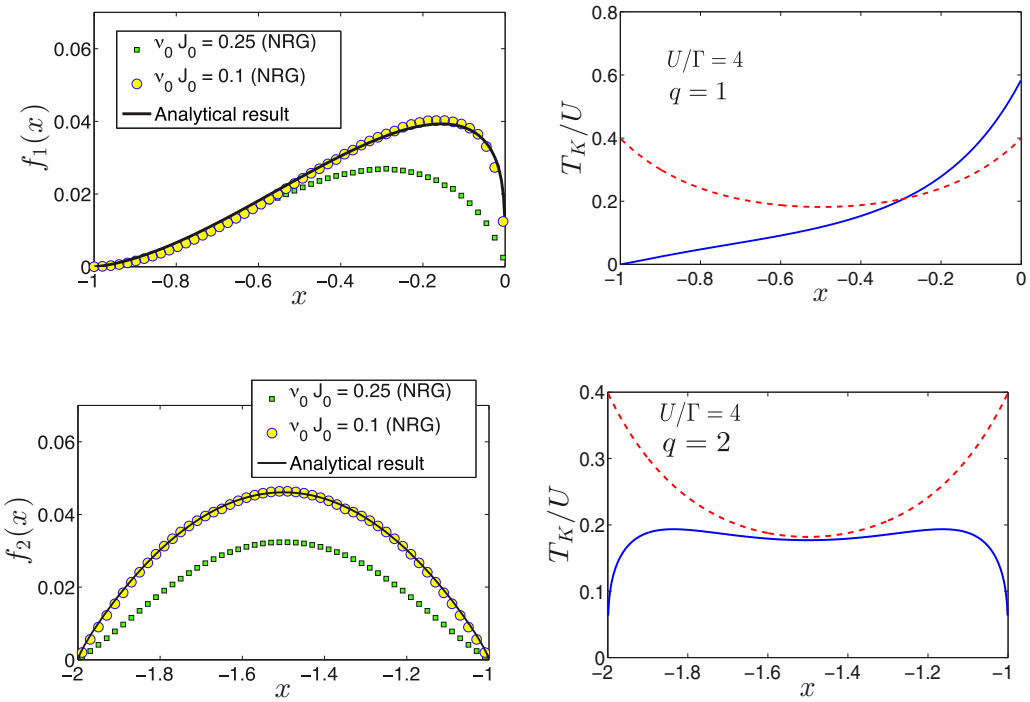

FIG. 2. (Color online) (left panel) Comparison of the analytical prefactors $f_1(x)$ and $f_2(x)$ in Eq. (4) (solid lines) with $\mathcal{D}_{\rm eff}/U$, extracted from NRG calculations (symbols). The numerical calculations were carried out for $\nu_0 J_0 = \{0.1, 0.25\}$. The sector $q = 3$ is symmetric to that with $q = 1$: $f_3(x-3) = f_1(-x)$. (right panel) Comparison of T_K/U for $U/\Delta = 4$ with the effective cutoff of Eq. (4) (solid line) or a constant prefactor $\sqrt{2U\Delta/\pi}$ instead of $D_{\rm eff}\sqrt[4]{2\nu_0 J_0}$ in Eq. (3) (dashed line).

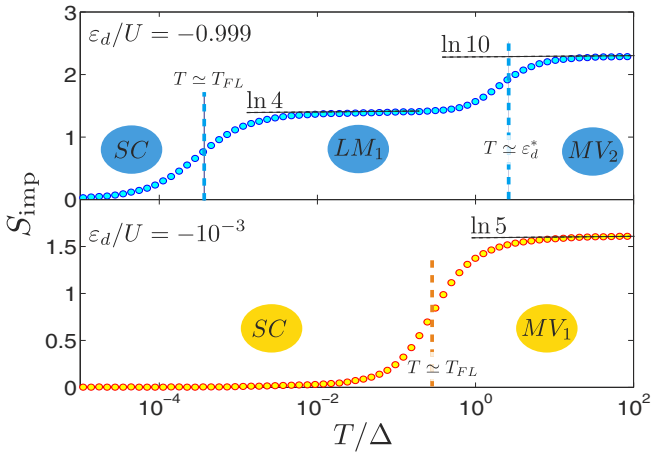

FIG. 3. (Color online) Temperature dependence of impurity contribution to the entropy.

the effects of valence fluctuations, which have a determining impact on the functions f_q and T_K; see Fig. 2.

To verify the analytical predictions, we also performed NRG computations by using the Budapest Flexible DM-NRG code [22] and compared the numerically obtained Kondo temperature to the analytical result, Eq. (4). As shown in Fig. 2, an excellent agreement is found for small values of $\nu_0 J_0$ [23]. Clearly, our results contradict the naive expectation that $\mathcal{D}$ should roughly correspond to the minimum charging energy of the quantum dot, in which case the edges of the functions f_q would exhibit a linear behavior. Rather, as discussed below, for small Δ the value of $\mathcal{D}_{\rm eff}$ is strongly renormalized by valence fluctuations. While for f_2, the discrepancy with linearity close to $x = -2$ and -1 is not very strong, it is much more pronounced for f_1 where, in addition, a strong asymmetry is observed. These differences are the results of the competition of different charge configurations in the vicinity of the mixed-valences regions MV_1 and MV_2 (see Fig. 1), as we discuss next.

Valence fluctuations. The importance of charge fluctuations is evident from the numerical study of the SU(4) Anderson model. Figure 3 displays the temperature dependence of the impurity entropy for two values of ϵ_d close to the $q = 0 \to 1$ and $q = 1 \to 2$ charge transitions, as determined by our DM-NRG computations. The impurity entropy $S_{\rm imp}(T)$ displays steps at each temperature corresponding to a "phase boundary" in Fig. 1. For $\epsilon_d \approx -0.001U$, e.g., the impurity entropy takes the value of $S_{\rm imp} = k_B \ln 5$ at high temperatures, corresponding to the approximate $(1 + 4)$-fold degeneracy of the $q = 0$ and $q = 1$ states (region MV_1), and by decreasing the temperature further below T_K, one enters directly the Fermi-liquid regime with $S_{\rm imp} = 0$. For $\varepsilon_d \approx -0.999\,U$, on the other hand, the entropy takes a value of $k_B \ln 10$ at hight temperatures, reflecting the $(6 + 4)$-fold degeneracy of the almost-degenerate $q = 2$ and $q = 1$ charging states (region MV_2), and a reduction series of $\ln 10 \to \ln 4 \to 0$ is observed, corresponding to the $MV_2 \to LM_1$ and $LM_1 \to$"Fermi-liquid" transitions.

From the previous analysis it is clear that, in the vicinity of the charging transitions, the mixed-valence fixed points govern the physics over a large energy window and have a substantial impact on quantum fluctuations—determining the precise Kondo scale. In fact, the basic structure of the functions f_q can be understood by means of a relatively simple renormalization group procedure constructed by Haldane [11], accounting also for charge fluctuations. Before proceeding with the full derivation of the functions f_q, let us present this simple and instructive derivation. We first consider the case $\Delta \ll -\varepsilon_d \ll U$ where the $q = 0$ and $q = 1$ states compete in region MV_1. In a standard renormalization group (RG) picture, ε_d is first renormalized by charge fluctuations in the region MV_1 and is replaced by

$$\varepsilon_d^* = \varepsilon_d + \frac{3\Delta}{\pi} \ln \frac{U}{\alpha|\varepsilon_d|} \tag{5}$$

in the region LM_1, with α a constant of order one. The factor 3 in Eq. (5) accounts for the balance between the empty state and the fourfold-degenerate singly occupied state. In region LM_1 (below a cutoff energy $\mathcal{D} \approx \alpha\varepsilon_d$), the QD can only be singly occupied, and a standard SU(4) Kondo effect takes place. The exchange constant J can be estimated here by the Schrieffer–Wolff approach because $J = -2\Delta/(\pi\varepsilon_d^*)$. Combining $\mathcal{D}$ and J within the two-loop expression of the Kondo temperature, we recover Eq. (3) with $\mathcal{D}_{\rm eff} = \sqrt[4]{\alpha|\varepsilon_d|U^3}/4$, yielding $f_1(x)|_{x\to 0^-} \propto \sqrt[4]{|x|}$ in agreement with the analytical expression of $f_1(x)$ (with $\alpha^{-1} = \gamma_e$ identified as Euler's constant). The reason for the emerging noninteger power is the logarithmic correction to ε_d, Eq. (5), which—after exponentiation in the Kondo temperature's expression—rescales the effective cutoff $\mathcal{D}_{\rm eff}$ to be of a nontrivial power-law form.

The same reasoning can be extended to the proximity of the region MV_2. Note that there are six different states with double occupancy. Each of them is coupled to two singly occupied states by the tunneling term, while each singly occupied state is coupled to three states with double occupancy. As a result we find $\mathcal{D}_{\rm eff}/U = \alpha^{5/4}(\varepsilon_d/U + 1)^{5/4}$ for $\varepsilon_d > -U$ and $\mathcal{D}_{\rm eff}/U = (\alpha|\varepsilon_d/U + 1|)^{3/4}$ for $\varepsilon_d < -U$ in agreement with the general expressions obtained for $f_1(x)$ and $f_2(x)$ (with again $\alpha = 1/\gamma_e$). The three limiting expressions derived so far by simple scaling arguments are sufficient to qualitatively understand the shape of the effective cutoff $\mathcal{D}_{\rm eff}$ shown in Fig. 2, in particular the strong asymmetry in f_1. In addition, these limits depend only on the orbital degeneracy and not on the details of the model at high energy. They have a universal character and apply also to systems which slightly break the SU(4) symmetry [24].

Path integral approach. To determine the functions f_q precisely, we must go beyond the previous simple analysis. The Schrieffer–Wolff (SW) transformation, applied to Eq. (1), gives the Kondo coupling J_0 of Eq. (3), but only a rough estimate of the cutoff $\mathcal{D}_{\rm eff}$. Moreover, any subleading correction to J_0 renormalizes $\mathcal{D}_{\rm eff}$. A precise determination of $\mathcal{D}_{\rm eff}$ thus requires a second-order calculation in Δ, or fourth order in the tunneling t, beyond SW. We follow the path integral approach devised in Ref. [16], where a systematic expansion in Δ is performed, and extend it to the SU(4) symmetry. Bosonic (fermionic) slave fields, associated with each even (odd) charged state of the QD, are introduced. They give a quadratic Anderson Hamiltonian at $t = \Delta = 0$ around which a diagrammatic perturbation theory in Δ is used. Below,

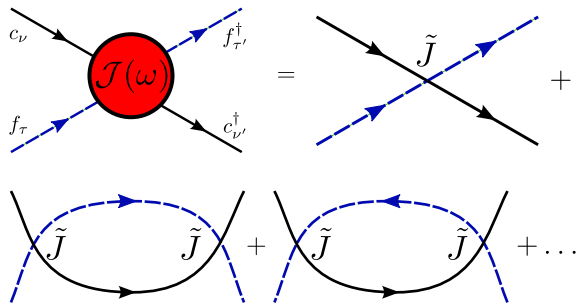

FIG. 4. (Color online) Diagrammatic expansion from Eq. (6) for the spin-exchange process $\mathcal{J}(\omega)$ to second order in Δ. Scattering lead electrons are considered at the energy ω, while slave fermions are considered at energy $\tilde{\varepsilon}_d$.

we focus on the case $q = 1$, but a similar discussion applies equally for the cases $q = 2$ and $q = 3$.

In the path integral formalism, the high-energy slave fields associated with QD states with $q \neq 1$ are integrated out, and the Anderson model is mapped onto a SU(4) Kondo-like action

$$S_{\rm K} = \sum_{\tau\tau'=1}^{4} {\rm Tr}\left[\frac{\tilde{J}}{2}\left(f^\dagger_{\tau'} f_\tau - \frac{1}{4}\right) c^\dagger_{k\tau} c_{k'\tau'}\right]. \tag{6}$$

The trace in Eq. (6) refers to summations over all wave vectors and Matsubara frequencies. In contrast to the genuine Kondo model, $\tilde{J}$ in Eq. (6) is a frequency-dependent coupling [16]. This dependence is a remainder of the integrated charge fluctuations in the Anderson model in addition to the Kondo-like spin fluctuations. To leading order in Δ and neglecting its frequency dependence, $\tilde{J}$ reduces to the SW coupling J_0. For energies ω below the charging energy U, dot excitations out of the $q = 1$ subspace are frozen and the Anderson model maps (for $-\varepsilon_d \gg \Delta$ and $\varepsilon_d + U \gg \Delta$) onto the Kondo model. The Kondo temperature $T_{\rm K}$ becomes the only relevant energy scale, which controls the Kondo crossover. As a result, the expansion of the exchange process $\mathcal{J}(\omega)$ in the Anderson model recovers exactly the same expansion as Eq. (2), derived within the Kondo model [see Eq. (7a)]. We can thus identify J and $\mathcal{D}$ from this weak-coupling expansion and determine $T_{\rm K}$.

Equipped with the action Eq. (6), we calculate the spin-exchange process $\mathcal{J}(\omega)$, given by the series of diagrams represented in Fig. 4. To be consistent with the second-order expansion in Δ, self-energy vertex corrections must also be considered. They lead to a renormalization of the orbital energy, analogous to Eq. (5), $\varepsilon_d \to \tilde{\varepsilon}_d = \varepsilon_d + \nu_0 t^2[\ln(-\varepsilon_d)/\Xi + 3\ln(\varepsilon_d + U)/\Xi]$, with Ξ denoting an UV regularization cutoff (to be distinguished from $\mathcal{D}$), eventually sent to infinity. The self-energy corrections also give rise to a *quasiparticle weight* $\mathcal{Z} = 1 + \nu_0 t^2[1/\varepsilon_d - 3/(\varepsilon_d + U)]$ for the slave fermions f_τ, which renormalizes the spin-exchange process. The complete calculation leads to the renormalized exchange amplitude,

$$\mathcal{J}(\omega) = J_0 + 2\nu_0 J_0^2 g_1\left(\frac{\varepsilon_d}{U}\right) - 2\nu_0 J_0^2 \ln\frac{\omega}{\mathcal{D}}, \tag{7a}$$

$$g_1(x) = \frac{1}{4}\frac{3x-2}{x+2} - \frac{x^2}{2}\frac{(x^2+3x+3)}{(x+2)^2}\ln\frac{2x+3}{x+1}, \tag{7b}$$

with $\mathcal{D} = [-\varepsilon_d(\varepsilon_d + U)^3]^{1/4}$. Comparison with Eq. (2) for $N = 4$ yields then the exchange coupling $J = J_0 + 2\nu_0 J_0^2 g_1(\varepsilon_d/U)$. Finally, computing the Kondo temperature $T_{\rm K,SU(4)}$, we obtain Eq. (3) with

$$f_1(x) \equiv \sqrt[4]{-x(x+1)^3}\exp[g_1(x)]. \tag{8}$$

As a result of the Kondo model renormalizability, different values of J and $\mathcal{D}$ can be chosen [25]. However, they all lead to the same Kondo temperature. The function $f_2(x)$ can be derived by a similar procedure. Details of its rather lengthy derivation as well as the analytical form of f_2 are given in the Supplemental Material [26].

Conclusions. In this work, we determined the Kondo temperature of the SU(4) Kondo model. In contrast to the SU(2) case, the prefactor of $T_{\rm K}$ was found to depend strongly on ϵ_d through universal functions of ϵ_d/U, which we determined analytically and numerically. As demonstrated through an analysis similar to that of Haldane, charge fluctuations play a decisive role in determining the aforementioned prefactors and lead to a power-law suppression of the Kondo scale close to the SU(4) mixed-valence fixed points. In addition to being of fundamental interest, the anomalous dependence of the Kondo temperature found here should be of importance when characterizing SU(4) Kondo systems. A study of the gate-voltage dependence could be performed similarly to SU(2) systems [2,27].

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