Low-energy physics of three-orbital impurity model with Kanamori interaction

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We discuss the low-energy physics of the three-orbital Anderson impurity model with the Coulomb interaction term of the Kanamori form which has orbital SO(3) and spin SU(2) symmetry and describes systems with partially occupied $t_{2g}$ shells. We focus on the case with two electrons in the impurity that is relevant to Hund’s metals. Using the Schrieffer-Wolff transformation we derive an effective Kondo model with couplings between the bulk and impurity electrons expressed in terms of spin, orbital, and orbital quadrupole operators. The bare spin-spin Kondo interaction is much smaller than the orbit-orbit and spin-orbital couplings or is even ferromagnetic. Furthermore, the perturbative scaling equations indicate faster renormalization of the couplings related to orbital degrees of freedom compared to spin degrees of freedom. Both mechanisms lead to a slow screening of the local spin moment. The model thus behaves similarly to the related quantum impurity problem with a larger SU(3) orbital symmetry (Dworin-Narath interaction) where this was first observed. We find that the two problems actually describe the same low-energy physics since the SU(3) symmetry is dynamically established through the renormalization of the splittings of coupling constants to zero. The perturbative renormalization group results are corroborated with the numerical-renormalization-group (NRG) calculations. The dependence of spin Kondo temperatures and orbital Kondo temperatures as a function of interaction parameters, the hybridization, and the impurity occupancy is calculated and discussed.

I. INTRODUCTION

The theoretical work of recent years has led to a considerably better understanding of the origin of electronic correlations in materials with wide bands and relatively weak Coulomb interactions, such as iron-based superconductors and ruthenates. Based on the dynamical mean-field theory calculations (DMFT) it has been realized that a small multiplet splitting coming from the Hund’s rule part of the Coulomb interaction ($J \ll U < W$, with $W$ the bandwidth, $U$ Hubbard interaction) has drastic effects at low energy scales.5–6 This has important consequences for the physics of these materials that are hence being referred to as the Hund’s metals.7,8

Impurity models play a major role in the DMFT studies since the problem of the bulk is mapped to a problem of a quantum impurity embedded in a self-consistently determined bath. It is interesting to note that whereas in the single-orbital setting the relevant impurity problem was well explored10 prior to the development of the DMFT, this is not the case for multi-orbital systems where the DMFT calculations preceded20 the detailed investigation of the impurity models upon which those calculations are based. The discovery of the strong influence of the Hund’s rule coupling within the DMFT has encouraged studies of multi-orbital effects also for adatoms on metal surfaces.11,12

In this paper we study the three-orbital impurity problem with Kanamori interaction

$$H_{\text{imp}} = \frac{1}{2}(U - 3J)N_d (N_d - 1) - 2JS^2 - \frac{J}{2}L^2,$$  \hspace{1cm} (1)

relevant for instance to the DMFT description of a transition-metal oxide with partially occupied $t_{2g}$ shells. In three-orbital systems, the physics of Hund’s metals occurs at occupancy $N_d = \frac{1}{2}$. $L, S$ are the orbital momentum and spin operators, respectively. Hamiltonian in Eq. (1) has a SU(2) spin and SO(3) orbital symmetry. The low-energy properties of the model defined by Eq. (1) have not been studied so far.

The effects of the Hund’s rule coupling were explored for several simpler (mostly two-orbital) models.11–22 The common conclusion of these works is that the Hund’s rule coupling suppresses the Kondo temperature through reduced exchange coupling of the low-lying impurity spin degrees of freedom with conduction electrons.

More recently, a Dworin-Narath (DN) impurity model23 was studied24–26. The DN model is described in terms of the simplified interaction Hamiltonian

$$H_{\text{imp}} = \frac{1}{2}(U - 3J)N_d (N_d - 1) - 2JS^2,$$ \hspace{1cm} (2)

which is similar to Eq. (1), but without the orbital part of the Hund’s interaction, $-(J/2)L^2$. The DN model has a higher SU(3) orbital symmetry and different fixed points. This work has led to important qualitative insights into the physics of Hund’s metal. Namely, Refs. 23–25 derived a Kondo Hamiltonian with a SU($M$) orbital and SU($N$) spin symmetry and argued that the key property is that the spin-spin Kondo coupling is ferromagnetic (or small) and that a two-stage screening of spin and orbital degrees of freedom occurs (see also an earlier pioneering study27). In Ref. 26 a renormalization group (RG) analysis stressed the importance of different spin and orbital degeneracy. These findings were corroborated by the numerical-renormalization-group (NRG) study in Ref. 26.

Given the deep implications of these results it is important to investigate the problem for the more realistic interaction term that is actually used in the DMFT calculations. In this paper we investigate the low-energy physics...
of the Anderson impurity model (AIM) with Kanamori interaction at occupancy close to \( N_d = 2 \) which is relevant to Hund’s metals. We derive the corresponding Kondo Hamiltonian using the Schrieffer-Wolff transformation. The distinction between the Kanamori and the Dworin-Narath Hamiltonian is found to become asymptotically irrelevant: at low energies, the orbital SO(3) symmetry is dynamically enlarged to the larger SU(3) symmetry. Consequently, the qualitative picture of the two-stage screening applies also for the Kanamori Hamiltonian. We also performed the NRG simulations that confirm these weak-coupling RG findings. We calculated the dependence of spin and orbital Kondo temperatures for a range of parameters and electron occupancies. Except at very low values of the Hund’s rule coupling strength, the spin Kondo temperature is significantly smaller (an order of magnitude or more). The smaller bare value of the spin-Kondo coupling as well as its slower running both contribute to such behavior.

The paper is structured as follows. In Sec. II we start with the description of the model. In Sec. III we present the Schrieffer-Wolff transformation, the resulting Kondo Hamiltonian, and the Kondo couplings. In Sec. III C we discuss the RG flow using the poor man’s scaling approach. In Sec. IV we give the NRG results. In Sec. V we conclude with a discussion of the implications of our results and with prospects for future work. In appendices A and B we give technical details on the derivation of Kondo Hamiltonian and RG flow, respectively. In appendix C we express the Kondo Hamiltonian in terms of rescaled couplings in a way that the couplings and the scaling equations are equal when the Hund’s coupling is zero. In appendix D we compare the behavior of Dworin-Narath and Kanamori models.

II. IMPURITY MODEL

The impurity models of interest to this paper can be written in the following way:

\[
H_{\text{bath}} = \sum_{k,m,\sigma} \epsilon_k c_{km\sigma}^\dagger c_{km\sigma}, \quad (3)
\]

\[
H_{\text{hyb}} = \sum_{k,m,\sigma} V_k c_{km\sigma}^\dagger d_{m\sigma} + \text{h.c.} = V \sum_{m,\sigma} c_{m\sigma}^\dagger d_{m\sigma} + \text{h.c.}, \quad (4)
\]

\[
H_{\text{imp}} = -2JS^2 - \frac{\alpha J}{2} L^2 + \frac{U - 3J}{2} N_d(N_d - 1) + \epsilon_0 N_d, \quad (5)
\]

with

\[
N_d = \sum_{m,\sigma} d_{m\sigma}^\dagger d_{m\sigma},
\]

\[
S = \sum_{m,\sigma} \left( \frac{1}{2} \sigma_{\sigma'} \right) d_{m\sigma'},
\]

\[
L = \sum_{\sigma} d_{m\sigma}^\dagger c_{mm'd_{m'\sigma}}.
\]

The operators \( c_{m\sigma}^\dagger \) and \( d_{m\sigma}^\dagger \) annihilate (create) bath and impurity electrons with spin \( \sigma = \pm 1 \) in orbital \( m \in \{1, 2, \ldots, M\} \), \( M \) being the number of orbitals. The non-interacting conduction electrons (\( H_{\text{bath}} \)) have energy \( \epsilon_k \), which corresponds to a flat density of states \( \rho_0 = 1/2D_0 \) with half-bandwidth \( D_0 \). In the hybridization function (\( H_{\text{hyb}} \)) we use the notation \( \sum_k V_k c_{km\sigma} = V c_{m\sigma} \). The hybridization strength is defined as \( \Gamma = \pi \rho_0 V^2 \).

The interaction of the electrons on the impurity is described by the term \( H_{\text{imp}} \) where we introduced the parameter \( \alpha \) that tunes the impurity interaction between Dworin-Narath (\( \alpha = 0 \)) and the Kanamori (\( \alpha = 1 \)) case in a continuous way. We will refer to the impurity model above as the Anderson impurity model (AIM) to distinguish it from the Kondo model defined in the following. \( N_d \) is the total impurity charge operator, \( S \) is the total impurity spin operator (\( \sigma \) are Pauli matrices), and \( L \) is the total impurity orbital angular momentum (\( L \) are spin-1 matrices for \( M = 3 \)). The spin and orbital momentum operators obey the Lie algebra commutation relations and are normalized such that

\[
\text{Tr}(X^\alpha X^\beta) = 2 \delta_{\alpha,\beta}, X \in \{L, S\}.
\]

In the following section we derive an effective Kondo Hamiltonian for the simplest realistic model that captures the Hund’s physics: the three orbital (\( M = 3 \)) AIM with two electrons or holes occupying the impurity such that the ground state orbital moment and spin are \( L = 1, S = 1 \).

We choose units such that \( D_0 = 1, k_B = 1, g\mu_B = 1 \).

III. KONDO HAMILTONIAN AND RG ANALYSIS

A. Schrieffer-Wolff transformation

To investigate the low-energy behavior of coupled bath and impurity electrons we derive an effective Kondo Hamiltonian in which the charge fluctuations on the impurity are suppressed. This is achieved using the canonical Schrieffer-Wolff transformation. The interaction term that is induced by virtual fluctuations from the ground-state impurity multiplet into the high-energy manifolds with \( n \pm 1 \) electrons reads

\[
H_K = -P_n H_{\text{hyb}} \left( \sum_a \frac{P^n_a}{\Delta E_{n+1}^{a+1}} + \sum_b \frac{P^n_b}{\Delta E_{n-1}^{a-1}} \right) H_{\text{hyb}} P_n.
\]
Projector operators $P_a$ project onto the atomic ground state multiplet with valence $n$. Projectors $P^{\pm 1}_{a+1}$ project onto the high energy multiplets having energy $E_{n+1}^a$ (indices $a, b$ denote different invariant subspaces with respect to $H_{imp}$) and the virtual excitation energies are $\Delta E_{n+1}^a = E_{n+1}^a - E_n^a$; $E_n$ is the ground state energy.

For the case of Kanamori Hamiltonian, Eq. (7) can be rewritten (see Appendix A for the derivation) in the following “Kondo-Kanamori” form:

$$H_K = J_p N_f + J_s S \cdot s + J_L L \cdot l + J_Q Q \cdot q + J_{gs} (L \otimes S) \cdot (l \otimes s) + J_{qs} (Q \otimes S) \cdot (q \otimes s).$$  (8)

$N_f$ is the bulk electron charge operator at the position of the impurity, $S, L, Q (s, l, q)$ are total impurity (bath) spin, orbital, and orbital quadrupole operators, respectively. The Kondo Hamiltonian contains besides spin-orbit and orbital quadrupole operators second order orbital tensor operators depending on the impurity, $S, L, Q (s, l, q)$ are total impurity (bath) spin, orbital, and orbital quadrupole operators, respectively. The five (symmetric and traceless) quadrupole matrices are the Gell-Mann matrices.

In this expression, $Q_{i, j}$ is the total bath spin operator and $t^a = \sum m' n' \epsilon^a_{m n} \gamma_{m n} \delta_{m' n'}$, $\epsilon^a_{m n}$ are the Gell-Mann matrices. $S$ and $T$ are the generators of spin-1 representation of SU(2) and the fundamental representation of SU(3).

The total set of eight generators $\{L, Q\}$ is, in fact, equivalent to the set of SU(3) generators $\{T\}$: both sets constitute a basis for traceless Hermitian $3 \times 3$ matrices.

The five (symmetric and traceless) quadrupole operators are second order orbital tensor operators defined as

$$Q_{i, j} = \frac{1}{2} \left( L_{i, m} L_{m, j} + L_{i, m} (t^b_{m, j}) - \frac{2}{3} \delta_{b, c} \delta_{i, j} \right).$$  (9)

For the more symmetric AIM with Dwarin-Narath interaction, the corresponding Kondo Hamiltonian reads

$$H_K^{DN} = J_p N_f + J_s S \cdot s + J_L L \cdot l + J_Q Q \cdot q + J_{gs} (L \otimes S) \cdot (l \otimes s) + J_{qs} (Q \otimes S) \cdot (q \otimes s).$$  (11)

In this expression, $S$ is the total bath spin operator and $t^a = \sum m' n' \epsilon^a_{m n} \gamma_{m n} \delta_{m' n'}$, $\gamma^a_{m n}$ are the Gell-Mann matrices. $S$ and $T$ are the generators of spin-1 representation of SU(2) and the fundamental representation of SU(3).

These bare Kondo couplings are presented in Fig. 1(b) for different values of the parameter $b$. The spin-spin coupling $J_s$ is substantially smaller than others for most values of $b$ and changes sign on approaching $b = 1$ that corresponds to the regime of valence fluctuations between $N_d = 2$ and $N_d = 3$ (at the degeneracy point between

$$\epsilon_0 = \frac{3 + 2a}{2} J - (1 + b) [U - J (4 - a)].$$  (12)

It is measured from the Fermi level. The parameter $b \in [0, 1]$ controls the occupancy of the impurity before the projection to the $N_d = 2$ subspace and determines the potential scattering term of the Kondo Hamiltonian. The term is written so that when $b \to 0$ and $b \to 1$ the atomic $N_d = 2$ ground state becomes degenerate with the atomic lowest states with occupancies $N_d = 1$ and $N_d = 3$, respectively. The excitation energies $\Delta E_{1, 2}$ to states with impurity occupancy $N_d = 1, 2$ are presented in Table I. Superscripts $a, b, c$ denote the three multiplets with charge $N_d = 3$ having different values of spin and orbital moment.

### Table I. Excitation energies.

| Index | $N_d$ | $L$ | $S$ | $\Delta E$ |
|-------|-------|-----|-----|------------|
| $\Delta E_1$ | 1 | 1 | 1/2 | $b(U - (4 - a)J)$ |
| $\Delta E_3$ | 3 | 0 | 3 | $(1 - b)(U - (4 - a)J)$ |
| $\Delta E_3$ | 3 | 2 | 1 | $(1 - b)U + J(b(4 - a) + 2(1 - a))$ |
| $\Delta E_5$ | 3 | 1 | 1 | $(1 - b)U + J(b(4 - a) + 2)$ |

We note in passing that under the particle-hole transformation, not only the potential scattering term but also the spin-orbital coupling and the quadrupole-quadrupole coupling terms of the Hamiltonian in Eq. (8) are odd. As a result, the two-fold hypercharge degeneracy discussed in Ref. [3] does not apply even in the absence of potential scattering.

Next we calculate the Kondo coupling constants by comparing matrix elements of Hamiltonians in equations (7) and (8):

$$J_p = \frac{V^2}{18} \left( \frac{6}{\Delta E_1 - \Delta E_3^b} - \frac{4}{\Delta E_3^a} - \frac{5}{\Delta E_3^c} - \frac{3}{\Delta E_3^d} \right),$$  (13)

$$J_s = \frac{V^2}{18} \left( \frac{6}{\Delta E_1 - \Delta E_3^b} + \frac{2}{\Delta E_3^b} + \frac{5}{\Delta E_3^a} \right),$$  (14)

$$J_l = \frac{V^2}{12} \left( \frac{6}{\Delta E_1 + \Delta E_3^a} - \frac{5}{\Delta E_3^a} + \frac{3}{\Delta E_3^d} \right),$$  (15)

$$J_q = \frac{V^2}{12} \left( \frac{6}{\Delta E_1} + \frac{4}{\Delta E_3^b} + \frac{5}{\Delta E_3^c} - \frac{3}{\Delta E_3^d} \right),$$  (16)

$$J_{ls} = \frac{V^2}{6} \left( \frac{6}{\Delta E_1 + \Delta E_3^b} + \frac{4}{\Delta E_3^a} - \frac{1}{\Delta E_3^d} + \frac{3}{\Delta E_3^c} \right),$$  (17)

$$J_{qs} = \frac{V^2}{6} \left( \frac{6}{\Delta E_1} + \frac{4}{\Delta E_3^b} - \frac{1}{\Delta E_3^a} + \frac{3}{\Delta E_3^d} \right).$$  (18)

In the zero bandwidth limit, $V \to 0$, the impurity energy level which determines the impurity occupancy reads:

$$\epsilon_0 = \frac{3 + 2a}{2} J - (1 + b) [U - J (4 - a)].$$  (12)
This results from the different energies of the L and L\textsuperscript{\textastix} orbitals that control the charge fluctuations, \(\alpha\) the Hund’s coupling \(J\) for constant \(U_{\text{eff}} = U - 3J = 2, b=0.5\).

\(N_d = 2\) and \(N_d = 3\), the atomic average occupancy is 30/13 \(\approx 2.3\), while at the degeneracy point between \(N_d = 2\) and \(N_d = 1\), the atomic average occupancy is 8/5 \(\approx 1.6\). All couplings diverge on approaching the end points \(b = 0\) and \(b = 1\) where the cost for the charge excitations vanishes. The Kondo model and the derived couplings for the \(N_d = 2, L = 1, S = 1\) atomic ground state configuration cease to be valid there.

The results are qualitatively similar to those found for the Dworin-Narah model in Refs. [24] and [25] with the distinction that for the Kanamori model the orbital and quadrupole couplings are split:

\[
\begin{align*}
J_q - J_l &= \Delta J/2, \\
J_{qs} - J_{ls} &= -\Delta J
\end{align*}
\]

with

\[
\Delta J = V^2 \left( \frac{1}{\Delta E_3^2} - \frac{1}{\Delta E_3^2} \right) = \frac{2JoV^2}{\Delta E_3^2\Delta E_3^2}.
\]

This results from the different energies of the \(L = 1\) and \(L = 2\) three-electron spin-doublet multiplets, caused by the \(-\alpha(J/2)L^2\) term in the Hamiltonian. For the Kanamori model with \(\alpha = 1\) the splitting is largest when the Hund’s coupling reaches

\[
J = \frac{(1 - b)U}{\sqrt{9b^2 + 6b}}. \tag{19}
\]

For two electrons at the impurity \((b \approx 1/2)\) this occurs for \(J = 0.22U\). Fig. (1b) shows how the splitting develops as the Hund’s coupling \(J\) is increased from zero, while keeping the parameter that controls the charge fluctuations, \(U_{\text{eff}} = U - 3J\), constant. In other words, as \(J\) is varied, the Hubbard repulsion \(U\) is adjusted so that the effective impurity repulsion \(U_{\text{eff}} = E(3) + E(1) - 2E(2) = U - 3J\) is kept fixed; here \(E(N)\) denotes the energy of the lowest multiplet with occupancy \(N\). The splittings of Kondo couplings are initially linear in \(J\), but then slowly fall off as \(1/J\).

C. Poor man’s scaling analysis

We now discuss the low-energy physics of the derived Kondo-Kanamori Hamiltonian within the weak-coupling RG approach.\footnote{31} The scaling functions \(\beta_i = dJ_i/d\ln(D)\) describe the renormalization of the coupling constants as the half-bandwidth \(D\) is progressively reduced. To the lowest order they read:

\[
\begin{align*}
\beta_p &= 0, \tag{20} \\
\beta_s &= -\frac{1}{9} \left( 3J_{ls}^2 + 5J_{qs}^2 + 9J_s^2 \right), \tag{21} \\
\beta_l &= -\frac{1}{16} \left( 4J_l^2 + 3J_{ls}^2 + 5(4J_q^2 + 3J_{qs}^2) \right), \tag{22} \\
\beta_q &= -\frac{3}{8} \left( 4J_l J_q + 3J_{ls} J_{qs} \right), \tag{23} \\
\beta_{ts} &= \frac{1}{6} \left( 3J_t J_l + 5J_{ts} J_{ls} + 12J_{ts} J_s + 15J_q J_{qs} \right), \tag{24} \\
\beta_{qs} &= -\frac{1}{12} \left( J_{qs} (18J_l + 7J_q + 24J_s) + 3J_{ls}^2 + 18J_{ts} J_q \right). \tag{25}
\end{align*}
\]

For a particle-hole symmetric band (as is the case for the flat density of states, \(\rho_0 = 1/2\), used here) the potential scattering operator is marginal, \(\beta_p = 0\).

The symmetry of the Hamiltonian is reflected in the scaling equations. For instance, for vanishing Hund’s orbital coupling in the AIM, the initial orbital and quadrupole coupling constants in Eq. (13) are equal \(J_q = J_l\) and \(J_{qs} = J_{ls}\). For such SU(3) orbitally symmetric choice of bare coupling constants, the respective scaling functions coincide: \(\beta_q = \beta_l, \beta_{qs} = \beta_{ls}\) and hence \(J_q = J_l\) and \(J_{qs} = J_{ls}\) also after RG scaling.

It is interesting to omit the cross-terms by setting \(J_{ls} = J_{qs}\) which is preserved also after RG flow. Hence, the spin and orbit coupling constants undergo a separate scaling in this case. From the ratio of the two scaling functions: \(\beta_l/\beta_s = 3/2J_l^2/J_s^2\) one sees that besides the
larger bare value of $J_l$ additional factor $3/2$ (the ratio of the orbital and spin degeneracy) helps the faster renormalization of orbital couplings. This behavior, associated with the larger SU(3) symmetry holds only in the case of $J_q = J_l$.

When Hund’s coupling is zero, $J = 0$, the symmetry is enlarged further and the model becomes the Coqblin-Schrieffer (CS) model with SU(6) symmetry. In this case, all the coupling constants are simply related to each other and can be expressed in terms of a single constant $J_{CS} = 3J_a = 2J_l = J_{ls}$. The simple relation holds also for scaling functions $3\beta_s = 2\beta_l = \beta_{ls}$. (The integer factors could also be absorbed in the definition of the coupling constants. See Appendix C.)

We numerically solved the scaling equations for three characteristic cases. We display the results in Fig. 2. The top panels show the Kondo couplings and the bottom panels the scaling functions $\beta$ divided by the spin scaling function $\beta_s$.

In left-most panels (a, b) we set the initial values to those of the SU(6) symmetric case $3J_a = 2J_l = 2J_q = J_{CS} = 1$ but we suppressed the cross-terms and set $J_{ls} = J_{qs} = J_{CS}/100$. This illustrates nicely the slower running of the spin coupling that holds until the cross-terms become large. From this point on, the values of constants and hence the flow approach that of the Coqblin-Schrieffer SU(6) symmetric case.

Middle panels (c, d) display the effects of the splitting between the orbit and quadrupole terms. We used the Coqblin-Schrieffer values $3J_a = 2J_l = J_{ls} = J_{CS} = 1$ for all but the quadrupole and spin-quadrupole coupling constants that we suppressed $J_q = J_l/100$, $J_{qs} = J_{ls}/100$. When the quadrupole terms are small they can be neglected from the scaling equations Eq. (21)-(25). In this case initially the scaling of the spin coupling is faster than the scaling of the orbit coupling, because the normally large contribution of the quadrupole terms $J_{q,qs}$ to $\beta_l$ is not present. Only when $J_{q,qs}$ become comparable to $J_{ls}$, the renormalization of the orbital coupling becomes faster than the renormalization of the spin coupling and the ratio $\beta_l/\beta_s$ approaches $3/2$. It is important to note that the splitting between the orbit and quadrupole and spin-orbit and spin-quadrupole terms disappears at low energies.

This is also seen in panels (e, f) that show the behavior for realistic set of initial coupling constants corresponding to the Anderson model (with parameters $U = 3.2$, $J = 0.4$, $\Gamma = 1$). One sees that the already initially weak splitting between orbital and quadrupole terms disappears on approaching the low energies (best seen in inset to (e) that displays the ratio of the two). Thus the multiplet splitting due to orbital interaction in the Anderson model becomes insignificant at low energies. The SU(3) and SO(3) symmetric models describe the same low-energy physics. Similar dynamical symmetry generation (or restoration) has been observed in a number of other quantum impurity models as well.

IV. NUMERICAL RENORMALIZATION GROUP RESULTS

Using the NRG technique we solve the Kanamori, Dworin-Narath (DN), and the Kondo impurity model. The NRG results validate the qualitative insights from the poor man’s scaling approach discussed above. The
two-stage screening behavior with the spin being screened at a temperature that is significantly lower than that for the orbital moment occurs in all three models.

We have implemented an NRG code with conserved quantum numbers \((Q, S, T)\), corresponding to total charge, total spin and total orbital angular momentum, i.e., using the \(U(1)\otimes SU(2)\otimes SO(3)\) symmetry. This allows to perform three-orbital calculations even with modest computation resources.

A. Comparison between Dworin-Narath, Kanamori, and Kondo-Kanamori results

In Fig. 3 we present the temperature dependence of the effective spin and orbital moments, \(\chi_{S, L} T\), where \(\chi_{S, L}\) are the impurity orbital and spin susceptibilities. The Kanamori results are compared to those for the Kondo model with exchange couplings set by Eqs. (20)-(25) and those for the more symmetric Dworin-Narath model. At high temperatures, the results for different models significantly differ due to different high-energy physics. Nevertheless, at lower temperatures the different models behave alike. In particular, the Kondo-Kanamori curves are close to the Kanamori ones (the differences become even smaller if the ratio of the interaction to the hybridization is diminished) which validates our analytical approach. The Dworin-Narath model behaves similarly, the main distinction being noticeably higher screening temperature of the orbital moments.

In the inset to Fig. 3 we present the spin and orbital susceptibilities. The former is scaled by 1/4 for easier comparison. The spin susceptibility is much larger than the orbital susceptibility and the latter saturates at higher temperatures. This again shows faster screening of orbital degrees of freedom. The orbital susceptibility has a weak maximum before saturating to the low-temperature value. Similar behavior was found in earlier work.

To confirm the asymptotic equivalence of the models, we present in Fig. 4 the finite size spectra calculated with NRG for the DN and the Kanamori impurity models as a function of the NRG step. The two spectra are the same at low energies, which shows that the two models have the same low-energy Fermi-liquid fixed point with excitation spectrum parametrized by the quasiparticle phase shift which is determined by the Friedel sum rule for fixed occupancy \(N_d = 2\).

B. Kanamori results at integer occupancy \(N_d = 2\)

We now discuss the Kanamori model in more detail. It is convenient to define the spin and orbital Kondo temperatures as the scale at which the respective effective moment diminishes below a constant. We take the constant to be 0.07 for spin and 0.07/(l+1)/s(s+1) for the orbital effective moments. The \(l, s\) are orbital moment and spin of electrons. It is of interest to know how the spin \(T_K^{\text{spin}}\) and orbital \(T_K^{\text{orb}}\) Kondo temperatures vary with the parameters of the Hamiltonian. We first discuss the results at an integer occupancy \(N_d = 2\).

In Fig. 5(a)–(c) we plot \(T_K^{\text{spin}}\) and \(T_K^{\text{orb}}\) as a function of the Hund’s rule coupling \(J\) for several hybridization strengths \(\Gamma\). When \(J\) is smaller than the Kondo scale of the \(J = 0\) model, \(T_K(J = 0) = T_K^0\), the moments are screened before the Hund’s coupling has effect. In this regime symmetry of the model becomes SU\((M\times N)\), hence only a single Kondo scale exists \(T_K^{\text{spin}} = T_K^{\text{orb}}\). The Kondo temperature dependence on \(J\) is initially slow, but becomes faster as \(J\) becomes larger than \(T_K^0\) as seen from Fig. 5(c). In addition, close to the \(J ∼ T_K^0\) point, \(T_K^{\text{spin}}\) becomes smaller than \(T_K^{\text{orb}}\). Unlike \(T_K^{\text{spin}}\) that decreases monotonously with \(J\), \(T_K^{\text{orb}}\) has a weak maximum at \(J\) above \(T_K(J = 0)\), which arises as a consequence of an interplay between the orbital, quadrupole and spin-orbital, spin-quadrupole interactions. This can be understood from the behavior of the coupling constants at
small $J$. Namely, upon expanding the Kondo couplings to first order in $J$ one sees that the orbital-orbital and quadrupole-quadrupole Kondo interactions increase with $J$, e.g. $J_1 = J_{1s}^0 + \alpha J$, while the other coupling constants decrease, e.g. $J_{1s} = J_{1s}^0 - \beta J$, where $\alpha, \beta > 0$ are positive constants.

It is interesting to look at the spin and orbit Kondo temperatures also as a function of hybridization $\Gamma$. In Fig. 5(d) we present the logarithms of $T_{K}^{\text{spin}}$ and $T_{K}^{\text{orb}}$ as a function of $\Gamma^{-1}$ for zero and non-zero value of Hund’s rule coupling. In the first case, the spin and orbit Kondo scales are the same for all $\Gamma$. Conversely, in the second case, the spin Kondo temperature is below the orbit Kondo temperature for all $\Gamma$. The leading exponential dependence on $\Gamma$ is the same for both $T_{K}^{\text{spin}}$ and $T_{K}^{\text{orb}}$, as seen from equal slopes of the lines. The slopes depend on the repulsion and are $-U_{\text{eff}}/c$ with (at $N_d = 2$) $c \approx 3$ for the zero-$J$ case and $c \approx 4$ for the finite-$J$ case. The difference is due to increased degeneracy of multiplets in the $J = 0$ case.

C. Kanamori results away from integer filling

We now turn to the results away from integer filling. In Fig. 6(a)–(f) we display the Kondo temperatures for several $\Gamma$ and $J$, still keeping $U_{\text{eff}} = 2$ fixed, as a function of the impurity occupancy $N_d$ in an interval around 2. The spin and orbital Kondo temperatures behave differently. $T_{K}^{\text{spin}}$ exhibit an overall diminishing trend as $N_d$ is increased towards half-filling ($N_d \approx 3$) with a shallow minimum at $N_d = 2$ that becomes less pronounced for larger $\Gamma$ where $\log T_{K}^{\text{spin}}$ is roughly linear in $N_d$. Conversely, $T_{K}^{\text{orb}}$ increases when occupancy is changed from $N_d = 2$ in both directions for all values of $\Gamma$.

The different behavior of both Kondo temperatures on approaching half-filling is due to the lowest states at $N_d = 3$ having large spin but vanishing orbital moment, $L = 0, S = 3/2$, thus the screening of the spin is strongly suppressed because of its large size, while the orbital moment is screened at a higher temperature. At half filling, the notion of orbital Kondo temperature becomes meaningless, as the orbital moment is zero also in the limit of vanishing hybridization. This distinction disappears for $J = 0$, see Fig. 6(g) where the results for zero and non-zero $J$ are shown in a broader range of $N_d$. For $J = 0$ the spin and orbit Kondo temperatures are the same.

On approaching small occupancies, $N_d \ll 1$, the Kondo temperatures rapidly increase and no distinction is seen between zero and non-zero $J$ cases in panel (g). When there is on average a single electron in the impurity the Hund’s coupling has no effect.

In Fig. 6(h) the ratio between the spin and orbital Kondo temperatures is shown. One sees that $T_{K}^{\text{orb}}/T_{K}^{\text{spin}}$ rapidly increases as $N_d$ is increased and at the occupancy $N_d = 2$ this ratio is about 10 and is further increasing as we approach half-filling.

V. CONCLUSION

We investigated the low-energy behavior of the Kanamori model in the RG and NRG approaches. We derived the appropriate Kondo model that is described in terms of spin, orbital, and quadrupole degrees of freedom. At low energies the splitting between the orbital and quadrupole coupling constants becomes insignificant, therefore similar behavior as for a Hamiltonian with a larger SU(3) symmetry can be expected. The NRG results confirm these poor-man’s scaling findings. In particular, both models have the same strong-coupling Fermi-liquid stable fixed point at low energies and approach this fixed point in a similar way (in the physically relevant parameter range). We calculated the dependence of the spin and orbital Kondo temperatures on interaction parameters, hybridization, and impurity occupancy. The orbital Kondo temperature is larger, thus orbital moments are quenched first as the temperature is lowered. This behavior starts to occur as soon as the Hund’s rule coupling
is increased above the Kondo temperature of the problem without the Hund’s rule coupling. The screening of the spin-moments occurs at a temperature that is about an order of magnitude smaller\cite{20}. The ratio of the orbital Kondo temperature to the spin Kondo temperature becomes particularly large as the impurity occupancy is increased towards half-filling. Our results demonstrate that the NRG is capable of treating problems with realistic three-orbital interactions. This method could hence be used in the DMFT calculations, too. Another interesting line of investigation is the analysis of the derived Kondo impurity model for parameters that do not correspond to the Anderson-type model. Our preliminary results reveal a rich phase diagram with several distinct non-Fermi-liquid phases.

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**Appendix A: Kondo Hamiltonian Derivation**

In this appendix we derive the Kondo Hamiltonian from the AIM with either Dworin-Narath or Kanamori interaction using the Schrieffer-Wolff transformation. Kondo Hamiltonian having SO(3) orbital and SU(2) spin symmetry was earlier written in terms of unit tensor operators in Ref\cite{20}. Kondo Hamiltonian having SU(M) orbital and SU(N) spin symmetry was derived in Ref\cite{20}.

The Schrieffer-Wolff transformation reads:

$$H_K = -P_n H_{hyb} \left( \sum_a \frac{P_{n+1}}{\Delta E_{n+1}} + \sum_b \frac{P_{n-1}}{\Delta E_{n-1}} \right) H_{hyb} P_n.$$  

(A1)

The projector operator $P_n$ projects onto the atomic ground state multiplet with occupancy $n = N_d$. The projectors $P_{n \pm 1}$ project onto the high-energy atomic multiplets having energy $E_{n \pm 1}$ (indices $a, b$ denote the different invariant subspaces with respect to $H_{imp}$, as presented in the main text) and the virtual excitation energies are $\Delta E_{n \pm 1} = E_{n \pm 1} - E_n$, $E_n$ being the ground-state energy.
We adopt the Einstein summation notation and for the sake of clarity we at first disregard all the constants (e.g. \( V^2/\Delta E \)). The projection operators to atomic multiplets transform as an identical representation under all symmetry transformations of the problem, hence the multiplet splitting of the excited states affects only the coupling constants (we write \( \Gamma = H_{hyb} \)):

\[
\sum_a \langle n | \frac{P_a}{\Delta E_{n+1}} | \Gamma | n \rangle = \sum_a \frac{1}{\Delta E_{n+1}} \langle n | \Gamma | n \rangle. \tag{A2}
\]

\(|n\rangle = P_n|\Psi_{LS}\rangle \) is the ground state with valence \( n \), orbital moment \( L \) and spin \( S \). The virtual charge excitation process conserves the impurity charge, thus \( P_n d_i^+ P_n = 0 \). The non-zero terms in the Kondo Hamiltonian are of the form:

\[
H_K' = P_n \Gamma P_n = P_n (c_i^\dagger d_i, d_i^\dagger c_k \sigma_k + \text{h.c.}) P_n \tag{A3}
\]

Next we insert an identity:

\[
c_i^\dagger d_i, d_i^\dagger c_k \sigma_k = (c_i^\dagger \delta_{i,k}, \sigma_i, d_i, d_i^\dagger) (d_k \sigma_k, \delta_{k,j}, \sigma_j, c_j), \tag{A4}
\]

and use the following group-theoretical relations:

\[
\delta_{i,j} \delta_{k,l} = \frac{1}{a} \delta_{i,k} \delta_{j,l}, \quad \text{SU}(m), \tag{A5}
\]

\[
\delta_{i,j} \delta_{k,l} = \frac{2}{a} (\tau^b)_{i,j} (\tau^b)_{k,l}, \quad \text{SO}(m). \tag{A6}
\]

The generators \( \tau, \sigma, T \) live in the defining (fundamental) representation of the SU(\( m \)), SO(\( m \)) symmetric Lie group, respectively. The constant \( a \) depends on the normalization of the generators Tr(\( T^a T^b \)) = \( a \delta_{a,b} \) (typically \( a = 2 \)). In the SU(2) case \( \sigma \) are the Pauli matrices and in the SU(3) case \( \sigma \) are the Gell-Mann matrices.

To obtain the Kondo Hamiltonian from the AIM with the Dworin-Narath interaction in terms of spin and orbital operators, we insert the identity \( [A6] \) into equation \( [A5] \) for the spin and orbital degrees of freedom (since both have SU symmetry). The relation \( [A5] \) leads to a result in which the dummy indices associated with the bulk operators \( c_{i,j} \) are independent from the indices associated with the impurity operators, and can be summed over to yield spin/orbital momentum operators. The Kondo Hamiltonian with the Dworin-Narath interaction reads:

\[
H_{K}^{DN} = J_p N_f + J_s S \cdot s + J_t T \cdot t + J_{ls}(T \otimes S) \cdot (t \otimes s). \tag{A7}
\]

Bath operators are defined as:

\[
\textbf{s} = \sum_m c_m^\dagger \frac{1}{2} \sigma \sigma' c_{m'}' \tag{A8}
\]

\[
\textbf{t} = \sum_{\sigma} c_{m} \tau_{mm'} \epsilon_{m'} \sigma. \tag{A8}
\]

\( \tau, \sigma \) are the Pauli and Gell-Mann matrices, respectively. \( S \) and \( T \) are the generators of spin-1 representation of SU(2) and the fundamental representation of SU(3).

On the other hand the relation \( [A6] \) does not decouple the bulk/impurity dummy indices due to the term \( \delta_{i,j} \delta_{j,l} \). However, this problematic term can be, for the 3-dimensional SO(3) symmetric group, rewritten as

\[
\delta_{i,j} \delta_{k,l} = \frac{1}{3} \delta_{i,k} \delta_{j,l} + \frac{1}{2} (\tau^c)_{i,j} (\tau^c)_{k,l} + \frac{1}{2} \delta_{i,j} \delta_{k,l}, \tag{A9}
\]

which does lead to the desired decoupling. Above we used the orbital quadrupole operators defined as

\[
Q^c_{ij} = \frac{1}{2} (T^c_{i,m} T^c_{j,m} + T^c_{i,m} T^c_{j,m} - \frac{2}{3} \delta_{c,e} \delta_{i,j}). \tag{A10}
\]

The projector \( P \) describes all the scattering events of electrons from the impurity to the band edges. The prefactor is \( 1/\Delta E = \rho/\delta D (E - D + \epsilon_k)^{-1} \approx \rho/\delta D |D|^{-1} \). We assume that the conduction band is wide. \( D \) is the half-bandwidth, \( E \) is the energy measured relative to the ground state of the conduction electron gas and can be neglected, \( \epsilon_k \) is the energy of electrons near the Fermi surface and can also be neglected relative to \( D \).

In the following we present a convenient way for calculating the second order corrections to the renormalized Hamiltonian using the completeness relations from the previous section. We will illustrate the procedure on the case of the spin-spin Kondo interaction term \( J S \cdot \sigma \) for a single orbital model with \( S = 1/2 \). First, we write the impurity operators in terms of the fermionic operators

\[
S^\alpha \rightarrow d_i^\dagger \sigma^\alpha_{ij} d_j, \tag{B2}
\]

with additional constraint \( d_i^\dagger d_i + d_i^\dagger d_i = 1 \). \( d_i^\dagger, d_i \) creates/annihilates an electron on the impurity with spin.
$i \in \{\uparrow, \downarrow\}$, $\sigma^\alpha$ are the Pauli matrices. The bulk electron spin operator is:

$$\sigma^\alpha \rightarrow c_i^\dagger \sigma^\alpha c_j. \quad (B3)$$

c_i, c_i creates/annihilates an electron with spin $i$ in the bulk. The spin-spin operators may be expressed in terms of Kronecker $\delta$ symbols using the following completeness relation:

$$\sum_\alpha (\sigma^\alpha)_{i,j} (\sigma^\alpha)_{k,l} = 2\delta_{i,k}\delta_{j,l} - \delta_{i,l}\delta_{j,k}. \quad (B4)$$

[For other operators, such as orbital, quadrupole, and mixed operators, one can derive similar expressions from Eqs. [A5], [A6], [A10].] After inserting the completeness relation we obtain:

$$J^2 \sum_{ijkl} (2\delta_{i,l}\delta_{k,j} - \delta_{i,j}\delta_{k,l})d_i^\dagger d_j c_k^\dagger c_l P \times$$

$$\times \sum_{mnop} (2\delta_{m,p}\delta_{o,n} - \delta_{m,n}\delta_{o,p})c_l^\dagger c_p =$$

$$= J^2 \sum_{ijkl} \sum_{mnop} A_{mnop}^{ijkl} P d_i^\dagger d_j d_m c_k^\dagger c_o c_p. \quad (B6)$$

The projector $P$ consists of two contributions:

$$P = \delta_{jm}(\delta_{lo} + \delta_{lp}). \quad (B7)$$

The first term $\delta_{jm}$ follows from the single-occupancy constraint of auxiliary fermions, while the second term $\delta_{lo} + \delta_{lp}$ describes the processes that involve scattering of electrons/holes to the upper/lower band edge. In the expressions one can use $c_{\alpha k}^\dagger c_{\alpha k} = 0$ for the electron states $k$ in the upper band edge that are assumed empty and $c_{\alpha k}^\dagger c_{\alpha k} = 1$ for the electron states $k$ at the lower band edge that are assumed filled.

Now we sum over the indices $m, o$ to eliminate Kronecker $\delta$ symbols that come from the projection operator. The contribution of the electron scattering to the upper band edge reads:

$$J^2 \sum_{ijkl} \sum_{np} A_{ijnp}^{kl} d_i^\dagger d_n c_k^\dagger c_p. \quad (B8)$$

Next we sum over the dummy indices $j, l$. The correction to the Kondo exchange reads:

$$J^2 \sum_{iknp} (-4\delta_{ip}\delta_{kn} + 5\delta_{in}\delta_{kp})d_i^\dagger d_n c_k^\dagger c_p =$$

$$= -2J^2 s \cdot \sigma + 3J^2 \sum_{iknp} \delta_{in}\delta_{kp}d_i^\dagger d_n c_k^\dagger c_p. \quad (B9)$$

This result has the same form as the initial exchange interaction with an additional potential scattering term. A contribution from the scattering to the lower band edge is obtained in a similar fashion; the exchange term is the same, while the potential scattering term has an opposite sign and therefore cancels out that in Eq. (B9) since we have assumed a particle-hole symmetric conduction band. We recover the standard $\beta$ function of the $S = 1/2$ Kondo model.

Similar approach can be used to tackle the multi-orbital problem. The scaling functions for a flat band, general number of orbitals $M$ and $N = 2$ are:

$$\beta_s = \frac{M(J_{ls}^2 - M(J_{ls}^2 + 2J_s^2)) - J_{qs}^2(M^2 - M - 2)}{2M^2}, \quad (B11)$$

$$\beta_l = \frac{1}{16} (-4J_l^2(M - 2) - 3J_s^2(M - 2) - (M + 2)(4J_q^2 + 3J_{qs}^2)), \quad (B12)$$

$$\beta_q = -\frac{1}{8}M(4J_lJ_q + 3J_sJ_{qs}), \quad (B13)$$

$$\beta_{ls} = -\frac{J_{ls}(M(J_l^2 - 4J_s) + J_{qs}(M^2 - 4)) + J_qJ_{qs}M(M + 2)}{2M}, \quad (B14)$$

$$\beta_{qs} = -\frac{2J_{ls}J_lM(J_l^2 + 4J_s) + J_{ls}M(J_{ls}^2 - M - 2) + 2J_qM) + J_q^2(M^2 + 2M - 8)}{4M}. \quad (B15)$$

When $\alpha = 0, J_q = J_l, J_{qs} = J_{ls}$ and results are the same as obtained in Ref.[17,25] for the model with SU(M) orbital symmetry.

**Appendix C: Rescaled Kondo Hamiltonian**

In the Coqblin-Schrieffer model the coupling constants are related to each other: $3J_{p,s} = 2J_{l,q} = J_{ls,qs}$. We introduce rescaled coupling constants: $\tilde{J}_{p,s} = 3J_{p,s}, \tilde{J}_{l,q} = 2J_{l,q}, \tilde{J}_{ls,qs} = J_{ls,qs}$. The Kondo Hamiltonian in terms of rescaled couplings reads:

$$H_K = \tilde{J}_{p}/3N_f + \tilde{J}_s/3S \cdot s + \tilde{J}_{l}/2L \cdot 1 + \tilde{J}_q/2Q \cdot q + \tilde{J}_{ls}(L \otimes S) \cdot (1 \otimes s) + \tilde{J}_{qs}(Q \otimes S) \cdot (q \otimes s). \quad (C1)$$
Hence the rescaled Kondo couplings are written in a more symmetric form:

\[ \tilde{J}_p = \frac{V^2}{6} \left( \frac{6}{\Delta E_1} - \frac{4}{\Delta E_3^b} + \frac{5}{\Delta E_3^c} - \frac{3}{\Delta E_3^a} \right), \]  
\[ \tilde{J}_s = \frac{V^2}{6} \left( \frac{6}{\Delta E_1} - \frac{2}{\Delta E_3^b} + \frac{5}{\Delta E_3^c} + \frac{3}{\Delta E_3^a} \right), \]  
\[ \tilde{J}_t = \frac{V^2}{6} \left( \frac{6}{\Delta E_1} + \frac{8}{\Delta E_3^b} - \frac{5}{\Delta E_3^c} + \frac{3}{\Delta E_3^a} \right), \]  
\[ \tilde{J}_q = \frac{V^2}{6} \left( \frac{6}{\Delta E_1} + \frac{8}{\Delta E_3^b} + \frac{1}{\Delta E_3^c} - \frac{3}{\Delta E_3^a} \right), \]  
\[ \tilde{J}_l = \frac{V^2}{6} \left( \frac{6}{\Delta E_1} + \frac{4}{\Delta E_3^b} + \frac{5}{\Delta E_3^c} - \frac{3}{\Delta E_3^a} \right), \]  
\[ \tilde{J}_{qs} = \frac{V^2}{6} \left( \frac{6}{\Delta E_1} + \frac{4}{\Delta E_3^b} - \frac{1}{\Delta E_3^c} + \frac{3}{\Delta E_3^a} \right). \]  

Notice that in the limit of vanishing Hund’s coupling \( J = 0, \Delta E_i = \Delta E \), and all the couplings are the same and so are the scaling functions:

\[ \tilde{\beta}_p = 0, \]  
\[ \tilde{\beta}_s = -\frac{1}{3} \left( 3\tilde{J}_p^2 + 5\tilde{J}_s^2 + \tilde{J}_{qs}^2 \right), \]  
\[ \tilde{\beta}_t = -\frac{1}{8} \left( \tilde{J}_t^2 + 3\tilde{J}_p^2 + 5 \left( \tilde{J}_q^2 + 3\tilde{J}_{qs}^2 \right) \right), \]  
\[ \tilde{\beta}_q = -\frac{3}{4} \left( \tilde{J}_q\tilde{J}_p + 3\tilde{J}_{ls}\tilde{J}_{qs} \right), \]  
\[ \tilde{\beta}_{ls} = \frac{1}{12} \left( 3\tilde{J}_l\tilde{J}_{ls} + 10\tilde{J}_{ls}\tilde{J}_{qs} + 8\tilde{J}_{ls}\tilde{J}_s + 15\tilde{J}_q\tilde{J}_{qs} \right), \]  
\[ \tilde{\beta}_{qs} = -\frac{1}{12} \left( \tilde{J}_{qs}(9\tilde{J}_l + 7\tilde{J}_{qs} + 8\tilde{J}_s) + 3\tilde{J}_s^2 + 9\tilde{J}_{ls}\tilde{J}_q \right). \]

Appendix D: Comparison between Kanamori and Dworin-Narath models

Using parameter \( \alpha \) (Eq. 5 in the main text) the impurity interaction can be continuously tuned between the Dworin-Narath (\( \alpha = 0 \)) and the Kanamori (\( \alpha = 1 \)) form. Even though the SO(3) orbital symmetry is dynamically restored to SU(3) at low energies and hence the behavior of the two models is similar there are quantitative differences that we illustrate here.

In Fig. 7 we present the spin and the orbit Kondo temperatures as a function of Hund’s coupling for different values of \( \alpha \). Overall a qualitatively similar behavior is found. At small hybridizations up to an order of magnitude difference is found for large \( J \). For small hybridization the spin Kondo temperature for Dworin-Narath is non-monotonic at large \( J \) which is not the case for the Kanamori model. The calculated Kondo temperatures there differ by an order of magnitude between the two models which can be important for realistic DMFT calculations where the quantitative agreement with experiments is desired. Despite the overall similarity of the Dworin-Narath and Kanamori results, the more realistic Kanamori interaction needs to be used there.

\[ \Delta E_i = \Delta E, \]
Figure 7. Spin and orbital Kondo temperatures as a function of Hund’s coupling $J$ for different values of parameter $\alpha$ ($\alpha = 0$ DN interaction, $\alpha = 1$ Kanamori interaction). Model parameters are $U_{\text{eff}} = 2, N_d = 2$.

[References mention various authors and journals related to quantum physics, Kondo effect, angular momentum theory, and related topics.]

The precise value depends on the parameters. The dominant exponential dependence on the Coulomb interaction parameters is, however, the same for the spin and orbital Kondo temperature.