# Magnetic impurity coupled to interacting conduction electrons

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(Received 24 August 1995; revised manuscript received 12 October 1995)

We consider a magnetic impurity which interacts by hybridization with a system of weakly correlated electrons and determine the energy of the ground state by means of a $1/N_f$ expansion. The correlations among the conduction electrons are described by a Hubbard Hamiltonian and are treated to the lowest order in the interaction strength. We find that their effect on the Kondo temperature, $T_K$, in the Kondo limit is twofold: first, the position of the impurity level is shifted due to the reduction of charge fluctuations, which reduces $T_K$. Secondly, the bare Kondo exchange coupling is enhanced as spin fluctuations are enlarged. In total, $T_K$ increases. Both corrections require intermediate states beyond the standard Varma-Yafet ansatz. This shows that the Hubbard interaction does not just provide quasiparticles, which hybridize with the impurity, but also renormalizes the Kondo coupling.

## I. INTRODUCTION

Recently, heavy-fermion behavior has been observed in the electron-doped cuprate $Nd_{2-x}Ce_xCuO_4$ $(0.1 \lesssim x \lesssim 0.2)$.[1] Below 0.3 K a linear specific heat $C_v = \gamma T$ is observed with a large Sommerfeld coefficient $\gamma \simeq 4$ J/( mole Nd $K^2$). In the same temperature regime, the spin susceptibility is found to be independent of the temperature and the Sommerfeld-Wilson ratio is of order unity. These are characteristic features of heavy-fermion excitations.[2] However, the characteristic low-energy scale of the order of 1 K which is associated with this behavior cannot be explained by applying the usual theory of the Kondo effect which assumes that the conduction carriers behave as free particles.[3] This is not too surprising because undoped $Nd_2CuO_4$ is an antiferromagnetic charge-transfer insulator instead of a metal,[4,5] despite one hole per unit cell. Upon doping the Nd ions are therefore coupling to a system of strongly correlated electrons[6,7] rather than to weakly or uncorrelated ones.

*Hamiltonian and Scaling.* In order to explain this new type of heavy-fermion behavior, it has therefore been proposed to include the correlations among the conduction electrons by including an on-site repulsion.[3,8] Thus, the total Hamiltonian

$$H = H_c + H_f + H_{cf} \tag{1.1}$$

goes beyond that of the single-site Anderson impurity model.[9] $H_c$ is a Hubbard Hamiltonian describing the conduction electrons

$$H_c = H_t + H_U,$$

$$H_t = \sum_{k,\sigma} \epsilon(k) c^\dagger_{k\sigma} c_{k\sigma}, \tag{1.2}$$

$$H_U = \frac{\tilde{U}}{2N_s} \sum_{kk'q,\sigma\neq\sigma'} :c^\dagger_{k+\delta\sigma} c_{k\sigma} c^\dagger_{k'-\delta\sigma'} c_{k'\sigma'}:.$$

$c^\dagger_{k\sigma}$ creates an electron with spin $\sigma$ and momentum $k$, $N_s$ is the number of lattice sites. The noninteracting dispersion is given by $\epsilon(k)$. $:\cdots:$ denotes normal ordering with respect to the Fermi sea $|\,\mathrm{FS}\rangle$ where all states below the Fermi momentum, $k_F$, are occupied. The magnetic impurity is assumed to contain one orbital (e.g., $4f$), which is either empty or singly occupied. Double occupancies are excluded because of the strong repulsion of electrons in that orbital. The energy of the $f$ orbital is then given by

$$H_f = \epsilon_f \sum_\sigma \hat{f}^\dagger_\sigma \hat{f}_\sigma, \tag{1.3}$$

where $\hat{f}^\dagger_\sigma = |\sigma\rangle\langle 0|$ are Hubbard operators forbidding a double occupancy of the impurity site and $\epsilon_f < 0$. The two subsystems are coupled by a local hybridization

$$H_{cf} = \frac{\tilde{V}}{\sqrt{N_s}} \sum_{k,\sigma} (\hat{f}^\dagger_\sigma c_{k\sigma} + c^\dagger_{k\sigma} \hat{f}_\sigma). \tag{1.4}$$

Taking a twofold degeneracy of the $f$ orbital ($\sigma = 1,2$), the model defined in Eqs. (1.1–1.4) corresponds[3] to the situation found in $Nd_{2-x}Ce_xCuO_4$ since the crystal-field ground state of Nd is a doublet.[10] In order to perform a systematic expansion we set $\sigma = 1 \ldots N_f$ and consider large $N_f$. This generalization deserves some comment: If the conduction electrons are uncorrelated ($\tilde{U} = 0$), this corresponds to treating an $N_f$-fold degenerate impurity which hybridizes with an $s$-wave conduction band. This is seen by expanding the conduction-electron states in partial waves about the impurity site and, assuming a spherically symmetric hybridization, only conduction electrons with the same total angular momentum are coupled to the impurity, while the others play a passive role and can be dropped.[11]

Due to the interactions among the conduction electrons this change of basis does not simplify the Hamiltonian (1.1). Nevertheless, we will consider the Hamiltonian in Eqs. (1.1–1.4) for $\sigma = 1 \ldots N_f$, which could be viewed as an SU($N_f$) generalization of the original model which has SU(2) symmetry. We thereby create an artificial model, which no longer corresponds to the physical situation of an $N_f$-fold degenerate impurity hybridizing with a correlated $s$ band. The ad-

 

antage in doing so is, however, that a controlled approximation becomes possible for this model, namely an expansion in $1/N_f$.[12]

In taking the limit $N_f \to \infty$, we keep the density of conduction electrons per spin constant, so that the kinetic energy increases $\propto N_f$. To have a proper limit $N_f \to \infty$, the hybridization coupling constant $\tilde{V}$ has to be scaled according to $\tilde{V} = V/\sqrt{N_f}$.[11] As regards the Hubbard interaction, we set $\tilde{U}/2 = U/(2N_f)$ as was suggested in Ref. 13. With this scaling, the correction to the ground-state energy of the Hubbard model (1.2) is of order $N_f^0$, both in second-order perturbation theory in $U$ and when summing the diagrams of the random-phase approximation (RPA), which is one order less than the $U=0$ energy.

*A straightforward variational ansatz.* In case the conduction electrons are uncorrelated ($U=0$) Varma and Yafet[14] proposed the following variational ansatz for the ground-state wave function of (1.1)

$$|\Psi_0\rangle = \left(1 + \sum_{q\sigma} \alpha_q \hat{f}_\sigma^\dagger c_{q\sigma}\right)|\mathrm{FS}\rangle. \tag{1.5}$$

$|\mathrm{FS}\rangle$ denotes the filled Fermi sea with empty $f$ level. Via $H_{cf}$, it couples to the states $f_\sigma^\dagger c_{q\sigma}|\,\mathrm{FS}\rangle$. Each of them describes a singlet formed between the $f$ level and the free electron state with momentum $q$, where $q$ is restricted to occupied states ($|q| \leqslant k_F$). Minimizing $\langle\Psi_0|H - E_S|\Psi_0\rangle$ with respect to $\alpha_q$ yields an approximate ground-state energy $E_S$. Compared to the energy $E_M$ of the multiplet $f_\sigma^\dagger|\mathrm{FS}\rangle$, this collective singlet formation gives rise to a gain in kinetic energy. With this energy gain a characteristic temperature scale $T_K$, the Kondo temperature, is associated. In the Kondo limit ($|\varepsilon| \ll D \ll |\epsilon_f|$, $2D =$ bandwidth) one finds[14] (in units of the bandwidth)

$$T_K = n\,\exp\left(\frac{\epsilon_f - \mu}{\rho V^2}\right). \tag{1.6}$$

Here we assumed a constant density of states $\rho = 1/(2D)$ of the conduction electrons. $\mu$ is the chemical potential of the conduction electrons and $n = (D+\mu)\rho$ denotes the filling per spin. Subsequently, it has been shown that in an expansion in the inverse degeneracy of the magnetic impurity, the ansatz (1.5) yields the ground-state energy to order $(1/N_f)^0$.[15]

In the case $U \neq 0$, it is, therefore, tempting to generalize the ansatz (1.5) by replacing the noninteracting ground state $|\mathrm{FS}\rangle$ by the (unknown) one of the Hubbard model, $|g\rangle$.[16] The expectation values with respect to $|g\rangle$ which arise in a variational calculation are given by the moments of the spectral function of the Hubbard model, which can be taken from, e.g., applying the projection technique.[16] If we assume Fermi-liquid behavior for the Hubbard model, the result of this generalized ansatz is obvious. We introduce quasiparticles $\tilde{c}^\dagger$ via $c_{q\sigma}^\dagger = \sqrt{Z}\tilde{c}_{q\sigma}^\dagger + \cdots$, where $Z$ denotes their renormalization factor. These quasiparticles hybridize with the impurity site rather than bare electrons, the effective hybridization being, however, renormalized by $\sqrt{Z}$. Therefore, we expect a Kondo temperature

$$T_K \propto \exp\left(\frac{\epsilon_f}{\rho_{\mathrm{QP}} Z V^2}\right), \tag{1.7}$$

where $\rho_{\mathrm{QP}}$ is the quasiparticle density of states at the chemical potential. Noting that $\rho = Z\rho_{\mathrm{QP}}$ is the many-particle density of states we see that the correlations enter only via $\rho$. In particular, $T_K$ is not modified for small $U$. This is in contrast to Ref. 17 where it has been shown for the Kondo model by a mean-field decoupling that due to polarization effects the Kondo temperature increases, even to lowest order in $U$. In the strongly correlated case Eq. (1.7) cannot be correct as well since the Kondo exchange coupling should be $V^2/U$ rather than $V^2/\epsilon_f$.[8]

To clarify the quality of the variational approach, we will restrict ourselves to the weakly correlated case in this paper and perform a $1/N_f$ expansion to lowest order in $U$. The theoretical framework, the Brillouin-Wigner perturbation series, is introduced in the next section. In particular, we will show that to order $1/N_f$ additional contribution arise from the Hubbard interaction in the singlet channel which do not occur in the multiplet channel (Sec. III) and conclude that these contributions modify the Kondo temperature. They are estimated in Sec. IV and the results are discussed in Sec. V.

## II. BRILLOUIN-WIGNER PERTURBATION THEORY

The $1/N_f$ expansion for the ground-state energy can be derived with the help of Brillouin-Wigner perturbation theory:[15,18,19] We decompose $H$ from Eq. (1.1) into $H_0 + H_1$ and choose $H_1 = H_U + H_{cf}$ as perturbation. In order to obtain the singlet ground-state energy we take as unperturbed ground state the filled Fermi sea $|\mathrm{FS}\rangle$. The energy $E_S$ of the ground state of $H$ (relative to the energy of $|\,\mathrm{FS}\rangle$) is given by[20]

$$E_S = \langle \mathrm{FS}|H_1 \sum_{n=0}^{\infty} \left(\frac{Q}{E_S - \tilde{H}} H_1\right)^n |\mathrm{FS}\rangle. \tag{2.1}$$

Here, $Q = 1 - |\mathrm{FS}\rangle\langle\mathrm{FS}|$ and $\tilde{H} = L_t + H_f$, where the Liouvillean $L_t$ is defined by $L_t A = [H_t, A]_-$. Equation (2.1) is equivalent to the zero-temperature limit of the equation for the lowest lying pole of the empty $f$-state propagator that appears in the partition function (see, e.g., Ref. 19).

*Diagrams.* The individual terms of the series (2.1) can be visualized by diagrams: In $H_1$, each $H_{cf}$ changes the occupation of the impurity level from 0 (wiggled line) to 1 (dashed line) destroying an conduction electron (solid line), since no double occupancy is allowed (and vice versa). This vertex carries a factor $V/\sqrt{N_f N_s}$. The impurity line changing always between occupied and unoccupied $f$ level constitutes the backbone of a diagram. $H_1$ contains $H_U$ as well. The vertex $H_U$ has two incoming and two outgoing conduction-electron lines. It yields a factor $U/(N_f N_s)$ and a $\delta$ function ensuring momentum conservation. Taking the expectation value with respect to $|\mathrm{FS}\rangle$ we connect the conduction-electron lines in all possible ways. The resolvent $Q/(\varepsilon - \tilde{H})$ yields the energy of the intermediate states and, because of the Liouvillean $L_t$ only the energy difference with respect to the filled Fermi sea enters. Conduction-electron lines pointing to the right correspond to particlelike excitations (with a momentum denoted by a capital letter, $|Q| > k_F$) while those pointing to the left are holelike (denoted by $|q| \leqslant k_F$). Without Hubbard interaction $H_U$ these

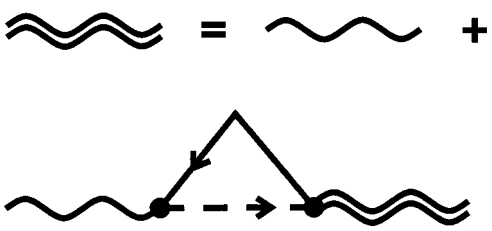

FIG. 1. Renormalization of the empty state propagator to order $(1/N_f)^0$.

rules correspond to the standard ones[11,19] for the self-energy of the propagator of the empty state in the partition function at zero temperature.

For an expansion in $1/N_f$ we note that each closed loop of fermions yields a summation over spin and, hence, a factor $N_f$, whereas each $V$ vertex is $\propto 1/\sqrt{N_f}$. To lowest order in $1/N_f$, the application of $H_U$ does not change the order of a diagram: If we connect two conduction-electron lines of a closed loop by the four-point interaction $H_U$ we create two loops with the only restriction $\sigma \neq \sigma'$, which is of higher order in $1/N_f$.

*Multiplet energy.* Similarly to Eq. (2.1), we obtain the energy $E_M$ for the multiplet ground state by taking the expectation values with respect to the multiplet state $f_\sigma^\dagger|\mathrm{FS}\rangle$. The resulting equation corresponds to the lowest pole of the propagator of the occupied $f$ state. The important energy for the low-temperature thermodynamics is given by the energy difference of singlet and multiplet ground state, $E_M-\mu-E_S$, which is related to the Kondo temperature.[21] Note that the multiplet has one electron more than the singlet in our definition.

*Renormalization of the bare propagators.* Already to order $(1/N_f)^0$ the bare empty $f$ level (single wiggle line, $1/z$) has to be renormalized [double wiggle line, $G_0(z)$]. This renormalization arises from a partial summation in Eq. (2.1) shown in Fig. 1:

$$G_0(z)=\frac{1}{z}+\frac{1}{z}I^{(0)}(z)G_0(z)=\frac{1}{z-I^{(0)}(z)}. \tag{2.2}$$

The self-energy $I^{(0)}(z)$ [see also Fig. 2(a)] evaluates to

$$I^{(0)}(z)=\frac{V^2}{N_s}\sum_q \frac{1}{z+\epsilon_q-\epsilon_f}. \tag{2.3}$$

The propagator of the occupied $f$ state, $G_1(z)$, is not renormalized to this order,

$$G_1(z)=\frac{1}{z-\epsilon_f}. \tag{2.4}$$

## III. GROUND-STATE ENERGIES TO ORDER $1/N_F$

*Diagrams for the singlet energy.* To order $(1/N_f)^0$ only the diagram shown in Fig. 2(a) occurs. It was already evaluated in Eq. (2.3)

$$I^{(0)}(z)=\frac{V^2}{N_s}\sum_q G_1(z+\epsilon_q). \tag{3.1}$$

There are no diagrams $\propto U$ to this order. To order $1/N_f$ we first find the diagram shown in Fig. 2(b):

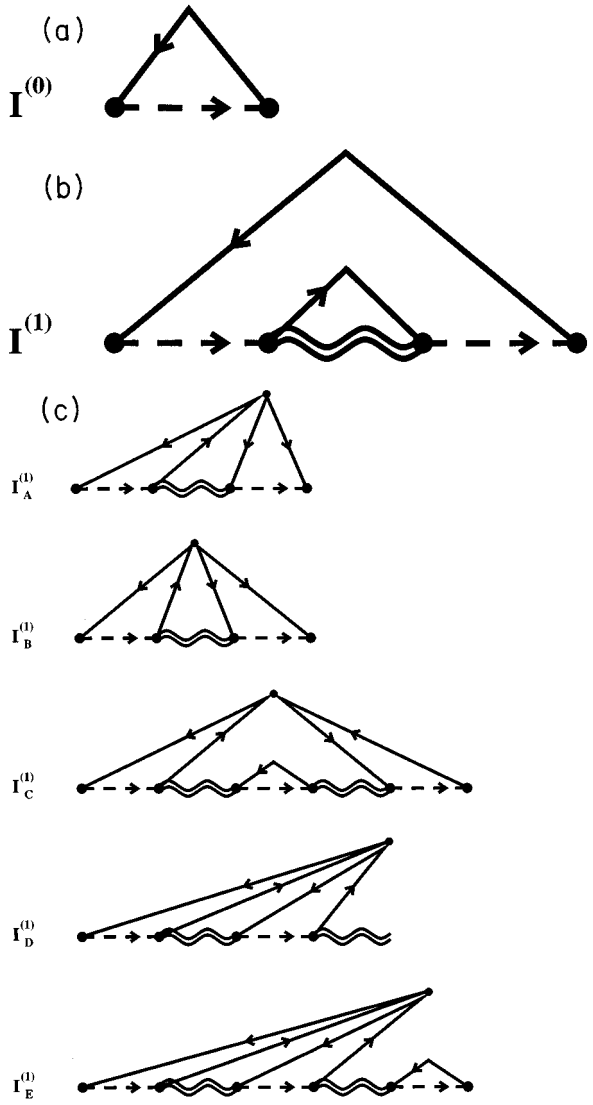


FIG. 2. Diagrams for the singlet ground-state energy. (a) Order $U^0$ and $(1/N_f)^0$, $I^{(0)}(z)$. (b) Order $U^0$ and $(1/N_f)^1$, $I^{(1)}(z)$. (c) Order $U^1$ and $(1/N_f)^1$, $I_i^{(1)}(z)(i=A,\ldots,E)$.

$$I^{(1)}(z)=\frac{V^4}{N_f N_s^2}\sum_{qQ}[G_1(z+\epsilon_q)]^2 G_0(z+\epsilon_q-\epsilon_Q). \tag{3.2}$$

As mentioned previously, applying $H_U$ does not change the order of a diagram to lowest order in $1/N_f$. Therefore, $I^{(1)}$ can be regarded as parent diagram in which we insert vertices of the interaction, $H_U$. Thereby we restrict ourselves to first order in $U$, i.e., we apply $H_U$ only once in the series (2.1). We then find the diagrams shown in Fig. 2(c). As the diagrams are time ordered, $I_A^{(1)}$ differs from $I_B^{(1)}$, etc. Also, applying $H_U$ over a doubly wiggled line deserves some comment (see, e.g., $I_B^{(1)}$): Such a diagram would not be unambiguous since it is not clear whether $H_U$ acts while the $f$ level is empty or occupied, when we expand the renormalized empty $f$ propagator as in Fig. 1. For that reason we define that $H_U$ acts while the (bare) $f$ level is empty. The other case yields a different diagram (here, $I_C^{(1)}$). The contributions of the diagrams of Fig. 2(b) are given by

$$I_A^{(1)}(z)=-\frac{2UV^4}{N_f N_s^3}\sum_{qrr'R} G_1(z+\epsilon_q)G_1(z+\epsilon_r+\epsilon_{r'}-\epsilon_R)G_0(z+\epsilon_r-\epsilon_R)G_1(z+\epsilon_r)\delta_{r'-q,R-r},$$

$$I_B^{(1)}(z)=\frac{UV^4}{N_f N_s^3}\sum_{qrQR} G_1(z+\epsilon_r)G_0(z+\epsilon_r-\epsilon_R)G_0(z+\epsilon_q-\epsilon_Q)G_1(z+\epsilon_q)\delta_{q-Q,r-R},$$

$$I_C^{(1)}(z)=\frac{UV^6}{N_f N_s^4}\sum_{qrr'QR} G_1(z+\epsilon_r)G_0(z+\epsilon_r-\epsilon_R)G_1(z+\epsilon_r+\epsilon_{r'}-\epsilon_R)G_1(z+\epsilon_q+\epsilon_{r'}-\epsilon_Q)G_0(z+\epsilon_q-\epsilon_Q)$$
$$\times G_1(z+\epsilon_q)\delta_{q-Q,r-R},$$

$$I_D^{(1)}(z)=\frac{2UV^4}{N_f N_s^3}\sum_{qrQR} G_0(z+\epsilon_q+\epsilon_r-\epsilon_Q-\epsilon_R)G_1(z+\epsilon_q+\epsilon_r-\epsilon_R)G_0(z+\epsilon_r-\epsilon_R)G_1(z+\epsilon_r)\delta_{Q-q,r-R},$$

$$I_E^{(1)}(z)=\frac{2UV^6}{N_f N_s^4}\sum_{qrr'QR} G_1(z+\epsilon_{r'})G_1(z+\epsilon_q+\epsilon_r+\epsilon_{r'}-\epsilon_Q-\epsilon_R)G_0(z+\epsilon_q+\epsilon_r-\epsilon_Q-\epsilon_R)G_1(z+\epsilon_q+\epsilon_r-\epsilon_Q)$$
$$\times G_0(z+\epsilon_q-\epsilon_Q)G_1(z+\epsilon_q)\delta_{Q-q,r-R}. \tag{3.3}$$

According to Eq. (2.1), the ground-state energy (relative to $E_{\rm FS}$) is given by the smallest solution of

$$E_S=I^{(0)}(E_S)+I^{(1)}(E_S)+\sum_{i=A}^{E} I_i^{(1)}(E_S). \tag{3.4}$$

There is no contribution $\propto UV^0$ in this expression for the ground-state energy since we introduced the Hubbard interaction in normal ordered form in Eq. (1.2) and restricted to first order in $U$. Hence the Hubbard interaction enters only via the hybridization $V$ in the ground-state energy. Expanding Eq. (3.4) in $1/N_f$ we obtain

$$E_S=E_S^{(0)}+\frac{1}{N_f}E_S^{(1)}+o(1/N_f)^2,$$

$$E_S^{(0)}=I^{(0)}(E_S^{(0)}),$$

$$E_S^{(1)}=\frac{I^{(1)}(E_S^{(0)})+\Sigma_{i=A}^{E} I_i^{(1)}(E_S^{(0)})}{1-\partial I^{(0)}(E_S^{(0)})/\partial E_{\rm S}}. \tag{3.5}$$

*Diagrams for the multiplet.* We now turn to the ground-state energy of a multiplet state. To order $(1/N_f)^0$ it is given by $E_M=\epsilon_f$ (relative to $E_{\rm FS}$). There is only one diagram contributing to order $1/N_f$, which is shown in Fig. 3. It is

$$J^{(1)}(z)=\frac{V^2}{N_f N_s}\sum_Q R_0(z-\epsilon_Q), \tag{3.6}$$

and we find therefore

$$E_M=\epsilon_f+J^{(1)}(\epsilon_f)+o(1/N_f)^2. \tag{3.7}$$


FIG. 3. Diagram for the multiplet ground-state energy, $J^{(1)}(z)$.

*Kondo temperature.* We associate the Kondo temperature, $T_K$, with the difference between singlet and multiplet ground-state energy[21] (in units of the bandwidth)

$$T_K=(E_M-\mu-E_S)\rho. \tag{3.8}$$

With this definition we find from Eqs. (3.5) and (3.7) to order $(1/N_f)^0$

$$T_K^{(0)}=(\epsilon_f-\mu)\rho-I^{(0)}(\epsilon_f-\mu-T_K^{(0)}/\rho). \tag{3.9}$$

Assuming a constant density of states we have

$$I^{(0)}(z)=\rho V^2\int_{-D}^{\mu} d\epsilon\frac{1}{z+\epsilon-\epsilon_f}$$
$$=\rho V^2\ln\left|\frac{(\epsilon_f-\mu)-z}{(D+\mu)+(\epsilon_f-\mu)-z}\right|, \tag{3.10}$$

and hence

$$T_K^{(0)}=(\epsilon_f-\mu)\rho-(\rho V)^2\ln\frac{T_K^{(0)}}{n+T_K^{(0)}}, \tag{3.11}$$

where $n=(D+\mu)\rho$ denotes the filling per spin. This is solved for small $J_K=-V^2/(\epsilon_f-\mu)$ by

$$T_K^{(0)}=n\,\exp\left(-\frac{1}{\rho J_K}\right), \tag{3.12}$$

cf. Eq. (1.6). To order $1/N_f$, we find from Eqs. (3.5), (3.7), and (3.8)

$$T_K^{(1)}=\rho\left[J^{(1)}(\epsilon_f)-\frac{I^{(1)}(E_S^{(0)})+\Sigma_{i=A}^{E} I_i^{(1)}(E_S^{(0)})}{1-\partial I^{(0)}(E_S^{(0)})/\partial E_S}\right]. \tag{3.13}$$

*Connection to variational approach.* To find the result (3.13) variationally the following states, which occur as intermediate states in the diagrams, have to be included in the trial state for the singlet ground state

$$\hat{f}^\dagger_\sigma c_{q\sigma}; c^\dagger_{Q\sigma} c_{q\sigma}; c^\dagger_{Q\sigma} c_{q\sigma} \hat{f}^\dagger_{\sigma'} c_{q'\sigma'} |\mathrm{FS}\rangle, \tag{3.14}$$

$$c^\dagger_{Q\sigma} c_{q\sigma} c^\dagger_{Q'\sigma'} c_{q'\sigma'}; c^\dagger_{Q\sigma} c_{q\sigma} c^\dagger_{Q'\sigma'} c_{q'\sigma'} \hat{f}^\dagger_{\sigma''} c_{q''\sigma''} |\mathrm{FS}\rangle. \tag{3.15}$$

The variational coefficients are determined up to first order in $U$ and to leading order in $1/N_f$.[16] In the free case ($U=0$) the first state corresponds to the ansatz of Varma and Yafet, cf. Eq. (1.5), which gives the result correctly to order $(1/N_f)^0$. The next two yield the $1/N_f$ corrections, while the last two are of order $(1/N_f)^2$.

## IV. ESTIMATING THE KONDO TEMPERATURE

In this section, we estimate the effect of the diagrams $\propto 1/N_f$ on the Kondo temperature. We scale the energies by $\rho$ and study the dependence on $T_K^{(0)}$ rather than on $E_S^{(0)}$ as $T_K^{(0)}$ is the small quantity. The transformed propagators read

$$\begin{aligned} i(x) &= -\frac{1}{\rho V^2} I^{(0)}(E_S^{(0)} - x/\rho) = \ln\left(\frac{x+n+T_K^{(0)}}{x+T_K^{(0)}}\right), \\ g_1(x) &= -\frac{1}{\rho} G_1(E_S^{(0)} - (x/\rho - \mu)) = \frac{1}{T_K^{(0)}+x}, \\ g_0(x) &= -\rho V^2 G_0(E_S^{(0)} - x/\rho) \\ &= \frac{\rho^2 V^2}{x + T_K^{(0)} - \rho(\epsilon_f - \mu) - \rho^2 V^2 i(x)} \end{aligned} \tag{4.1}$$

and depend implicitly on $T_K^{(0)}$ and $n$. The empty-state propagator, $g_0(x)$ diverges $\propto T_K^{(0)}/x$ for $x \to 0$. [This corresponds to the spin-fluctuation peak at $z = E_S^{(0)}$ in $G_0(z)$.] This singularity yields contributions $\propto T_K^{(0)} (\ln T_K^{(0)})^\nu$ to $I^{(1)}$, $I_i^{(1)}$, and $J^{(1)}$, which we neglect against terms which remain constant as $T_K^{(0)} \to 0$. For larger $x$ however, $g_0(x)$ drops slower than $1/x$ resulting in finite contributions. In this intermediate $x$ range ($T_K^{(0)} \ll x \ll n$), we may safely approximate

$$g_0(x) \sim \rho J_K \tag{4.2}$$

for small $T_K^{(0)}$. The validity of this replacement for the whole $x$ range in the diagrams has been checked numerically.

*Diagrams of order $U^0$.* We begin with the contributions $\propto U^0$ in Eq. (3.13)

$$I^{(1)}(E_S^{(0)}) = -\frac{\rho V^2}{N_f} \int_0^n du \int_0^{1-n} dx \; g_1^2(u) g_0(u+x), \tag{4.3}$$

$$J^{(1)}(\epsilon_f) = -\frac{1}{\rho N_f} \int_0^{1-n} dx \; g_0(x - T_K^{(0)}), \tag{4.4}$$

where we again assumed a constant density of states. Inserting (4.2) we find for the multiplet energy

$$J^{(1)}(\epsilon_f) = -\frac{J_K}{N_f}(1-n), \tag{4.5}$$

where the corrections are of higher order in $1/(\epsilon_f - \mu)\rho$. For the singlet energy we use the same approximation for $g_0$ to obtain

$$I^{(1)}(E_S^{(0)}) = \frac{(\rho V)^2 J_K}{N_f}(1-n)\left(\frac{1}{n+T_K^{(0)}} - \frac{1}{T_K^{(0)}}\right). \tag{4.6}$$

Together with the denominator in Eq. (3.13)

$$1 - \frac{\partial I^{(0)}(E_S^{(0)})}{\partial E_S} = 1 - (\rho V)^2 \left(\frac{1}{n+T_K^{(0)}} - \frac{1}{T_K^{(0)}}\right) \tag{4.7}$$

and neglecting the 1, we find that both contributions $\propto U^0$ cancel. (Loosely speaking, these terms describe the energy gain due to hybridization with unoccupied states which is the same for multiplet and singlet state.)

*Diagrams of order $U$.* We continue with the estimation of the diagrams $\propto U$. The numerical evaluation of the sums $I_A^{(1)}, \ldots, I_E^{(1)}$ is difficult because of the $\delta$ functions, which ensure momentum conservation in the Hubbard interaction. Since we are interested only in the qualitative behavior, we may neglect them. This implies that the interaction $U$ acts only at the lattice site 0 with which the impurity hybridizes and corresponds to taking the limit of infinite dimensions.[22] Then the sums $\propto U$ in Eq. (3.3) read

$$\begin{aligned} I_A^{(1)}(E_S^{(0)}) &= \frac{2UV^2\rho^2}{N_f} \ln\left(\frac{T_K^{(0)}}{n+T_K^{(0)}}\right) \int_0^n du \int_0^{1-n} dx \; g_1(u) g_0(u+x) i(u+x), \\ I_B^{(1)}(E_S^{(0)}) &= \frac{U}{N_f}\left[\int_0^n du \int_0^{1-n} dx \; g_1(u) g_0(u+x)\right]^2, \\ I_C^{(1)}(E_S^{(0)}) &= -\frac{UV^2\rho^2}{N_f} \int_0^n du \; dv \int_0^{1-n} dx \; dy \; g_1(u) g_0(u+x) g_1(v) g_0(v+y) \frac{i(u+x) - i(v+y)}{u+x-(v+y)}, \\ I_D^{(1)}(E_S^{(0)}) &= \frac{2U}{N_f} \int_0^n du \; dv \int_0^{1-n} dx \; dy \; g_1(u) g_0(u+x) g_1(u+v+x) g_0(u+v+x+y), \\ I_E^{(1)}(E_S^{(0)}) &= -\frac{2UV^2\rho^2}{N_f} \int_0^n du \; dv \int_0^{1-n} dx \; dy \; g_1(u) g_0(u+x) g_1(u+v+x) g_0(u+v+x+y) \frac{i(u+v+x+y) - i(0)}{u+v+x+y}. \end{aligned} \tag{4.8}$$

For the integrals $I_A^{(1)}$, $I_B^{(1)}$, and $I_D^{(1)}$ it proves numerically sufficient to replace $g_0(x)$ as in Eq. (4.2) in the limit $T_K^{(0)}\to 0$. Then the following leading behavior for $T_K^{(0)}\to 0$ can be calculated analytically

$$I_A^{(1)}(E_S^{(0)})=\frac{UV^2\rho^2 C(n)}{N_f}\ln\left(\frac{T_K^{(0)}}{n}\right),$$

$$I_B^{(1)}(E_S^{(0)})=\frac{U}{N_f}(1-n)^2,$$

$$I_D^{(1)}(E_S^{(0)})=-\frac{UC(n)}{N_f}(1-n)\frac{1}{\ln T_K^{(0)}}\to 0 \qquad (4.9)$$

with $C(n)=-2[n\ln n+(1-n)\ln(1-n)]>0$. The integral $I_E^{(1)}$ simplifies since one integration can be performed

$$I_E^{(1)}(E_S^{(0)})=-\frac{2UV^2\rho^2}{N_f}\int_0^n du\ dv\int_0^{1-n}dx\ g_1(u)\times\frac{1}{i(u+x)-i(0)}g_1(u+v+x)\times\ln\left(\frac{u+v+x+1-n}{u+v+x}\right). \qquad (4.10)$$

By numerical evaluation, one finds that $I_C^{(1)}$ and $I_E^{(1)}$ remain finite as $T_K^{(0)}\to 0$. They are, however, small compared to $I_B^{(1)}$ as they have an additional prefactor $\rho^2V^2$. Keeping only diagrams $I_A^{(1)}$ and $I_B^{(1)}$ in Eq. (3.13), which corresponds to considering only the states (3.14) in a variational calculation, we obtain in the limit of small $T_K^{(0)}$

$$T_K^{(1)}=-\frac{T_K^{(0)}}{N_f}\left(\rho UC(n)\ln\left(\frac{T_K^{(0)}}{n}\right)+\frac{U}{\rho V^2}(1-n)^2\right)=\frac{T_K^{(0)}}{N_f}\left(\frac{U}{J_K}C(n)-\frac{U}{\rho V^2}(1-n)^2\right). \qquad (4.11)$$

The first contribution to $T_K^{(1)}$ is positive and, therefore, enhances the Kondo temperature. Since it depends on $U/J_K$ it is related to spin degrees of freedom. A similar contribution was found in Ref. 17 and it was attributed to the enhancement of spin fluctuations that result from the reduction of charge degrees of freedom when turning on $U$. The second contribution in Eq. (4.11) depends on $\rho V^2$ rather than $J_K$. It is related to charge degrees of freedom. A similar effect has been found in Ref. 8 and has been interpreted as the increase in energy of the virtual state in the spin-exchange process because in the virtual state a conduction site is doubly occupied. It decreases the Kondo temperature. However, in the limit $\rho|\epsilon_f-\mu|\gg 1$ that we considered throughout, the first term dominates: Overall we find an increase of the Kondo temperature.

This interpretation can be put onto more solid grounds by the following observation: If we would not scale the Hubbard interaction among the conduction electrons by $1/N_f$, the corrections due to $U$, $I_i^{(1)}(z)$, would be of the same order as $I^{(0)}$. Then the integral $I_B^{(1)}(z)$, which remains constant as $z\to 0$, would effectively shift the position of the $f$ level to $\epsilon_f^*$, whereas $I_A^{(1)}(z)\sim\ln z$ would renormalize the exchange coupling $V^2/\epsilon_f^*$ [cf. Eqs. (3.9) and (3.11)]. However, without scaling there would be contributions of higher order in $U$ which diverge as $N_f\to\infty$.

*Comparison to previous results.* In Ref. 17, a Kondo model ($N_f=2$) with correlated conduction electrons has been investigated to lowest order in the interaction strength $\tilde{U}$ by a mean-field decoupling of the Kondo-exchange interaction. The following increase of the Kondo temperature has been found

$$\frac{T_K(\tilde{U})}{T_K(0)}=\exp\left(\frac{\alpha}{\rho J_K(1+\alpha)}\right) \qquad (4.12)$$

with $\alpha=(3/2)\rho\tilde{U}\ln 2$. In contrast to our result (4.11), the increase of the Kondo temperature seems to depend exponentially on $\tilde{U}$. Note, however, that in our treatment the interaction had to be scaled by $1/N_f$. Scaling $\tilde{U}$ in Eq. (4.12) and expanding in $1/N_f$ yields the first term of our result (4.11) (with a factor ln2 for $N_f=2$ at half filling instead of 3/4 ln2).

The second term of Eq. (4.11), which describes the effective shift of the $f$ level, cannot be found in Ref. 17 because there the Kondo model has been investigated, where the charge degrees of freedom of the impurity have already been projected out. Therefore, $J_K$ in (4.12) is an effective coupling constant which depends on $U$.[8]

Without scaling the Hubbard interaction, all integrals would be of order $(1/N_f)^0$. As discussed above, the position of the $f$ level and the Kondo coupling constant are modified, and these corrections occur in the exponent as in Eq. (4.12).

## V. CONCLUSION

The aim of this paper was to investigate the influence of correlations among the conduction electrons on the Kondo effect. Lead by the situation prevailing in $Nd_{2-x}Ce_xCuO_4$, we proposed a model with a twofold degenerate impurity ($N_f=2$) which hybridizes with a correlated $s$ band and straightforwardly generalized it to arbitrary $N_f$. As discussed in the introduction, this generalization does not correspond to the physical situation of an $N_f$-fold degerate impurity hybridizing with a correlated $s$ band for $N_f>2$, in contrast to the uncorrelated case. Although artificial, we saw that this model allows for systematically studying the effects of the correlations on those diagrams which are usually considered in the uncorrelated case.

In particular, we assumed that the correlations are weak and calculated their effect on the Kondo temperature to lowest order in $1/N_f$. We found two competing effects: The first contribution is related to charge fluctuations. Because the energy of the virtual state in the spin-exchange process increases, the Kondo temperature is reduced. This corresponds effectively to a shift of the position of the $f$ level. A similar effect has been found in Ref. 8. The second contribution is related to the enhancement of spin fluctuations of the conduction electrons. The Kondo exchange coupling is effectively enhanced and the Kondo temperature increases. In the

Kondo limit the second contribution dominates the first one, so that we find in total an increase of the Kondo temperature for small $U$.

In our opinion, more interesting is that corrections to the Kondo temperature occur already to lowest order in the Hubbard interaction $U$. To obtain them in a variational approach, trial states are needed which in the uncorrelated case yield corrections to the ground-state energy which are of order $1/N_f$ (and higher). Thus, our result cannot be obtained by an ansatz of the Varma-Yafet type (1.5). This shows that the effect of the Hubbard correlations is more intricate than just to provide quasiparticles with a modified density of states at the Fermi surface which hybridize with the $f$ orbital as it was described by Varma and Yafet for the uncorrelated case, $U=0$.

If we wish to proceed to higher order in $U$, we note that to order $1/N_f$ only RPA-type diagrams contribute since each $U$ vertex carries a factor $1/N_f$, which has to be compensated by a spin summation, i.e., a closed loop of conduction electrons [in fact, the ground-state energy of the Hubbard model (1.2) to order $1/N_f$ is given by summing the diagrams of RPA type and neglecting the $\sigma \neq \sigma'$ constraint]. Only few more intermediate states will occur. This is, however, an artifact of our scaling of the Hubbard interaction and one expects that in a realistic model (without the restrictive scaling of $H_U$ and finite $N_f$) intermediate states with more and more excited electron-hole pairs contribute, the number of which increases with increasing order of $U$. Therefore, it seems questionable that a systematic $1/N_f$ treatment grasps the correct physics for realistic models of interacting conduction electrons in the limit of strong correlations.

## ACKNOWLEDGMENTS

The author has benefited from numerous discussions with Professor P. Fulde, Dr. G. Khaliullin, and Dipl.-Phys. K. Fischer.

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