Pseudofermion ferromagnetism in the Kondo lattices: a mean-field approach

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1 Introduction

Experimental investigations of heavy-fermion and other anomalous $4f$- and $5f$-compounds, which are treated usually as Kondo lattices, demonstrate that magnetic ordering is widely spread among such systems. There exist numerous examples of systems where “Kondo” anomalies in thermodynamic and transport properties coexist with antiferromagnetic ordering and/or strong spin fluctuations. There are also examples of Kondo ferromagnets: CeNiSb, CePdSb, CeSi$_x$, CeRu$_3$B$_2$, Sm$_3$Sb$_4$, NpAl$_2$ (see review and bibliography in [1–3]). The number of such materials gradually increases, including CePt [4], CeRu$_2$Ge$_2$ [5], CeAgSb$_2$, CeRu$_2$M$_2$X (M = Al, Ga; X = B, C) [7,8], CeRh$_2$B$_2$ [9], hydrogenated CeNiSn [10]. Among 2D-like systems, we can mention CeRuPO, a ferromagnetic Kondo lattice where LSDA + U calculations evidence a quasi-two-dimensional electronic band structure [11]. Recently ferromagnetic state with small magnetic moments was investigated for the Kondo systems CeRuSi$_2$ [12] and Ce$_3$Sb$_{1.5}$Ge$_{1.5}$ [13].

Owing to competition with the Kondo effect, ferromagnetism of the Kondo lattices has itself anomalous features (instability of magnetic state; small values of magnetic moment and magnetic entropy, negative paramagnetic Curie temperature, etc.) [1–3]. Unusual nature of Kondo systems on the border of magnetism was recently reviewed by Coleman [14]. Formation of the magnetic state, coexisting with the Kondo effect and possessing a small magnetic moment, was treated in references [1,2] within a scaling approach. However, this method is insufficient to describe quantitatively the ground state. An attempt was made to solve this problem on the basis of mean-field approximation [15,16] by using the pseudofermion representation for localized $f$-spins [17]. In this approach, the pseudofermions become delocalized and the system is described by an effective $s$-$f$ hybridization model (Sect. 2).

Unfortunately, only saturated ferromagnetic solutions were obtained in references [15,16] since the bare density of states was taken in the rectangular form. In the present paper we consider the formation of the Kondo ferromagnetism by detailed analysis and numerical solution of equations of the mean-field approximation for an arbitrary $\rho(E)$. In Section 3 we investigate the conditions for existence of the saturated (half-metallic) ferromagnetic solution, and in Section 4 for non-saturated (small moment) ferromagnetism. In Section 5 we present results of numerical calculations for a number of concrete two- and three-dimensional lattices.

2 The model

We start from the standard Hamiltonian of the $s$-$f$ exchange model

$$H = \sum_{k\sigma} \epsilon_k c_{k\sigma}^{\dagger} c_{k\sigma} - \sum_q J_q S_{-q} S_q + H_{\text{int}},$$

$$H_{\text{int}} = -I \sum_{i\sigma\sigma'} (S_i \sigma \sigma') c_{i\sigma}^{\dagger} c_{i\sigma'},$$

(1)

where $c_{k\sigma}^{\dagger}$ are conduction electron operators, $\epsilon_k$ is the bare electron spectrum, $S_i$ are operators for localized spins, $\sigma$ are the Pauli matrices, $I$ is the $s$-$f$ exchange parameter.

A number of papers (see, e.g., [18,19]) treat ferromagnetism in the periodic $s$-$d$($f$) model starting from the equation of motion method for the original Hamiltonian (1), so that the subsystems of the conduction electrons and $f$-spins remain uncoupled in Kondo’s sense.
However, for anomalous $f$-system where the Kondo compensation (singlet formation) should be considered in the zero order approximation, such an approach turns out to be inappropriate. Therefore we construct the mean-field approximation describing the Kondo ground state with the use of the Abrikosov pseudofermion representation for localized spins $S = 1/2$

$$S_i = \frac{1}{2} \sum_{\sigma \sigma'} f^\dagger_{i\sigma} \sigma_{\sigma'} f_{i\sigma'}$$  \hfill (2)

with the subsidiary condition

$$f^\dagger_{i\sigma} f_{i\sigma} + f^\dagger_{i\sigma'} f_{i\sigma'} = 1.$$  

Making the saddle-point approximation for the path integral describing the spin-fermion interacting system [17] one reduces the Hamiltonian of the $s$-$f$ exchange interaction to the effective hybridization term:

$$-J \sum_{\sigma \sigma'} c^\dagger_{i\sigma} c_{i\sigma'} \left( \sigma_{\sigma'\sigma} - \frac{1}{2} \delta_{\sigma'\sigma} \right) f^\dagger_{i} V c_{i} + c^\dagger_{i} V f_{i},$$  

where the vector notations are used

$$f^\dagger_{i} = \left( f^\dagger_{i\uparrow}, f^\dagger_{i\downarrow} \right), \quad c^\dagger_{i} = \left( c^\dagger_{i\uparrow}, c^\dagger_{i\downarrow} \right),$$  

$V$ is the effective hybridization matrix which is determined from a minimum of the free energy. In the ferromagnetic state we have [15,16]

$$H - \mu n = \sum_{k \sigma} \left[ \left( t_k - \mu \right) c^\dagger_{k\sigma} c_{k\sigma} + W_{\sigma} f^\dagger_{k\sigma} f_{k\sigma} \right]$$

$$+ V_{\sigma} \left( c^\dagger_{k\sigma} f_{k\sigma} + f^\dagger_{k\sigma} c_{k\sigma} \right) - \sum_{\sigma} V_{\sigma}^2 / 1$$  \hfill (4)

with

$$W_{\sigma} = W - \sigma J_0 \bar{S},$$  

$W$ being the energy of pseudofermion “$f$-level”, $J_0 = J(q = 0)$ the maximum Fourier transform of the Heisenberg interaction. Thus we reduce the periodic Kondo ($s$-$f$ exchange) model to an effective hybridization model with the spin-dependent parameters $W_{\sigma}$ (the $f$-level position with respect to the chemical potential $\mu$, which is of order of the Kondo temperature $T_K$) and $V_{\sigma}$ (the effective hybridization). The equations for these quantities are presented in Appendix.

The corresponding density of states (DOS) reads

$$N_{\sigma}(E) = \rho \left( 1 + \frac{V_{\sigma}^2}{(E - W_{\sigma})^2} \right) \left( E - \frac{V_{\sigma}^2}{E - W_{\sigma}} \right) \rho \left( \frac{E - V_{\sigma}^2}{E - W_{\sigma}} \right)$$  \hfill (5)

(where $\rho(E)$ ($0 < E < D$) is the bare DOS) and is shown in Figure 1. The total capacity of $N(E)$ band is twice larger than that of $\rho(E)$ band (i.e., unity per each hybridization subband), since it includes contributions from both conduction electrons and pseudofermions. One can see that $N(E)$ reproduces and enhances peculiar features of the bare band. For realistic (considerably smaller) $V$ values in the Kondo systems the enhancement can be stronger.

![Figure 1](image1.png)

Fig. 1. The picture of hybridization density of states for the cubic lattice in the nearest-neighbor approximation. For clarity, a large value of $V$ is taken. The dashed line is the bare density of states.

![Figure 2](image2.png)

Fig. 2. The partial spin-up (upper half) and spin-down (lower half) densities of states for the rectangular bare band ($W_1 = W_0$). The vertical line is the chemical potential for the HFM state. Note that the polarizations of conduction electrons and pseudofermions are opposite.

### 3 Half-metallic Kondo ferromagnetism

On treating ferromagnetic state, we restrict ourselves to the case where the conduction electron concentration $n < 1$ (the results for $n > 1$ are obtained by the particle-hole transformation).

First we discuss the half-metallic ferromagnetic (HMF) solution where the chemical potential lies in the energy gap for $\sigma = \uparrow$ (Fig. 2) so that

$$W_1 > V_{\uparrow}^2 / (D - \mu), \quad -V_{\uparrow}^2 / \mu < W_1 < V_{\uparrow}^2 / (D - \mu).$$  \hfill (6)

Since the capacity of the hybridization subband equals unity, we have

$$n^f_{\uparrow} \approx 1 - n/2, \quad n^f_{\downarrow} \approx n/2, \quad \bar{S} \approx (1 - n)/2$$

whereas the magnetization of conduction electrons is still small, $n_{\uparrow} \approx n_{\downarrow} \approx n/2$. In this state, each conduction electron compensates one localized spin due to negative sign of $s$-$f$ exchange parameter $I$, and the magnetic ordering is
owing to exchange interaction between non-compensated moments. Such a picture is reminiscent of the situation in the narrow-band ferromagnet in the Hubbard or s-d exchange model with large intrasite interaction (double-exchange regime). In our case the bare interaction is small, but effective interaction is large in the strong coupling regime.

It is worthwhile to mention here an alternative approach based on a Gutzwiller-type variational principle, which was used in reference [20] for low-dimensional Kondo lattices. This approach gives ferromagnetism only at large $|I|$ values (Nagaoka limit) which are beyond the Kondo physics (where a small scale of the Kondo temperature exists).

Using (A.20) and (A.21), the second condition in (6) can be rewritten as

$$-M(n)\frac{\mu(2n) - \mu}{\mu} < 1 - \frac{J_0(1 - n)}{W_0 Q(n)} < M(n)\frac{\mu(2n) - \mu}{D - \mu},$$

where $W_0$ corresponds to the paramagnetic phase, $J_0$ is the Heisenberg exchange interaction,

$$M(n) \equiv \left( \frac{V_1}{V} \right)^2 = \exp \left( \frac{1}{\rho} \int_0^D \frac{\rho(E)}{E - \mu} dE \right),$$

$$Q(n) \equiv \frac{W_1}{W_0} = \exp \left( -\frac{1}{\rho} \int_0^{\mu(n+1)} \frac{\rho(E) - \rho}{E - \mu} dE \right).$$

For the rectangular bare band ($\rho(E) = 1/D, 0 < E < D$) we have

$$M(n)|\mu(2n) - \mu|/(D - \mu) = 1, \quad Q(n) = 1,$$

and the left-hand inequality in (7) takes the form

$$j = J_0/W_0 < \frac{2}{n(1 - n)}.$$  

It is interesting that, as well as for a Heisenberg ferromagnet, the solution exists for any small $J_0$ and can be stabilized by arbitrarily small exchange energy (of course, the situation can become different provided that we take into account fluctuations and the corresponding contributions to the total energy).

The character of solutions can change for an arbitrary form of $\rho(E)$. To ensure the large energy gap for spin up states, it is required that $\rho(E)$ is not small in the interval $[\mu_{2n}, D]$ and this interval is not narrow. In particular, the condition (7) holds if the electron concentration is small, especially provided that $\rho(E)$ has square-root behavior near the band bottom ($M(n)$ becomes large owing to the factor of $1/\rho$). Thus for small $J_0$ the HFM solution can disappear in some concentration region, but becomes restored with increasing $J_0$.

On the other hand, for some bare DOS and $n$ (where $M(n)|\mu(2n) - \mu|/(D - \mu) > 1$) the HFM state can be formally retained for negative $J_0$. Indeed, since the spin up hybridization gap is larger because of renormalization of $V_\uparrow$, there can exist HFM solutions with positive $\bar{S}$ but negative spin splitting, $W_\uparrow < W_\downarrow$ (of course, they are not energetically favorable owing to $f$-$f$ exchange interaction). The situation is again connected with negative sign of s-f exchange parameter: polarization of conduction electrons is antiparallel to the moment of f-electrons, and occurrence of magnetization results in a redistribution of electron density.

Note that the picture of half-metallic magnetism is intimately related to hybridization character of the spectrum, as well as in intermetallic $d$-systems [21].

### 4 Weak Kondo ferromagnetism

Now we consider the ferromagnetic solution with small magnetization $\bar{S} < (1 - n)/2$ where the condition $W_\sigma > V_\sigma^2/(D - \mu)$ holds for both $\sigma$ and the Fermi level lies in the lower hybridization subband (below the energy gap), as well as in the non-magnetic case.

We have

$$\frac{J_0 \bar{S}}{W} = \frac{W_1 - W_\downarrow}{W_1 + W_\downarrow}$$

Taking into account renormalization of hybridization in our model (see Appendix), we derive the self-consistent equation for magnetization

$$\frac{J_0 \bar{S}}{W} = L(\bar{S}, n),$$

$$L(\bar{S}, n) = \tanh \left( \frac{1}{2\rho n} \int_{\mu(n + 1 - 2\bar{S})}^{\mu(n + 1 + 2\bar{S})} \frac{\rho(E) - \rho}{E - \mu} dE \right),$$

$$(\rho = \rho(\mu))$$

and the expression for the renormalized Kondo temperature ($f$-level energy)

$$W = W_0 P(\bar{S}, n),$$

$$P(\bar{S}, n) = \frac{1}{2} \sum_\sigma \exp \left( \frac{1}{\rho} \int_{\mu(\sigma + 1 - 2\bar{S})}^{\mu(\sigma + 1 + 2\bar{S})} \frac{\rho(E) - \rho}{E - \mu} dE \right).$$

The non-saturated solution is smoothly joined with the HMF solution of previous section at

$$n + 1 - 2\bar{S} = 2n, \quad n + 1 + 2\bar{S} = 2.$$

In terms of the quantity $W_0$,

$$W_0 \approx V_0^2/\delta n, \quad \delta n = \mu_{n+1} - \mu_n, \quad \mu_n = \mu(n),$$

(which is more convenient for constructing phase diagram) we have the equation

$$j \bar{S} = P(\bar{S}, n) L(\bar{S}, n), \quad j = J_0/W_0.$$  

Solutions with $\bar{S} \neq 0$ may occur if both the left and right-hand side of (11) are of order unity, i.e. $J_0 \sim W_0$. However,
in fact the conditions are rather restrictive (note that the situation is somewhat similar to Hubbard-I approximation where strong dependence of magnetism criterion on bare DOS occurs [22]). In particular, equation (11) has no non-trivial solutions for $\rho(E) = \text{const.}$: the magnetization can occur only due to energy dependence of $\rho$.

A necessary (but not sufficient) condition for existence of ferromagnetism with small $S$ is

$$k_n = \left. \frac{dL(S,n)}{dS} \right|_{S=0} = \frac{1}{\rho_{n+1} - \rho_n} > 0,$$

(14)

where $\rho_n = \rho(\mu_n)$, $\rho'_n = 1/(2\rho_n)$. Therefore, as compared to half-metallic ferromagnetism which is governed by the global behavior of $\rho(E)$, the small $S$ ferromagnetism criterion is determined by $\rho(E \approx \mu_{n+1})$. The situation for existence of small $S$ solutions is more satisfactory at larger $n$ (e.g., near half-filling) and in the presence of high narrow peaks (at the same time, such peaks influence weakly the conditions (7)).

The equation for the ferromagnetic phase at $S \to 0$ is $k = j$, so that the non-saturated solution starts from $j = k$. Provided that HMF solution exists for a given $n$, $S$ increases with decreasing $j$ up to the point where $\bar{S} = (1-n)/2$ (when $n+1 = 2S$) and the Fermi level reaches the upper edge of lower hybridization band, $j$ being finite at this point (the spin splitting $2J_0\bar{S}$ should remain finite). Thus this solution exists in a restricted (both from above and below) and even rather narrow $j$ interval.

The situation changes if HMF solution does not exist at given $n$. Then the non-saturated solution can exist at arbitrarily small $j$ and even in the unphysical $j < 0$ region where $\bar{S}$ reaches $(1-n)/2$ with increasing $j$. Such an unusual behavior (in particular, decrease of the moment with increasing $j$) is connected with a peculiar nature of the non-saturated solution. In this state we have two competing tendencies. The growth of exchange splitting $2J_0\bar{S}$ with $j$ drives the chemical potential into the energy gap, but the sharp pseudofermion peak prevents its own crossing and remains above the Fermi level (Fig. 3). Thus $\bar{S}$ should decrease.

In this connection, we can refer to discussion of a sudden jump of the Fermi surface and of an extra Kondo destruction energy scale for various phases in Kondo lattices [23].

The illustrations based on numerical solution are given in the next section. To consider qualitatively the solutions with small moments we can perform the expansion in $\bar{S}$.

$$L_n(\bar{S}) = k_n\bar{S} - a_n\bar{S}^3 + \ldots$$

$$a_n = \left[ \rho''_{n+1}/\delta_n - \rho'_{n+1}/\delta_n^2 \right.$$  

$$+ 2(\rho_{n+1} - \rho_n)/\delta_n^3 \left]/(12\rho_{n+1}) + b_n/2 \right.$$.

(15)

(16)

where the $\bar{S}$-cubic contributions which come from the expansion of the chemical potential are similar to those in the usual Stoner theory,

$$\mu(n+1+2\bar{S}) - \mu(n+1-2\bar{S}) = 2\bar{S}/\rho_{n+1} + b_n\bar{S}^3 + \ldots$$

$$b_n = (3\rho_{n+1}^2/\rho'_n - \rho''_n - \rho'_{n+1}/\rho''_{n+1})/3.$$  

(17)

Taking into account the renormalization of $W$,

$$P(S,n) = 1 - c_n\bar{S}^2,$$

(18)

c_n = \left[ (\rho_{n+1} - \rho_n)/\delta_n \right.$$

$$+ \rho'_{n+1}(1 - 2\rho_{n+1}/\rho_{n+1}) \left]/(2\delta^2\rho_{n+1}^2) \right.$$  

(19)

we can estimate the magnetic moment as

$$\bar{S} = \sqrt{(k_n - j)/(a_n + c_n k_n + k_n^3/3)}.$$  

(20)

Thus it is favorable for the small-moment ferromagnetism that $\rho''_{n+1} < 0$ and the derivatives are large in absolute value. For example, this takes place when there is a narrow peak in bare DOS at (or somewhat higher) $\mu_{n+1}$, so that magnetic ordering shifts the peak from the Fermi level. Under these conditions, magnetic ordering can occur near electron concentrations $n$ corresponding to the peak position $E_1$, i.e. $\mu_{n+1} \simeq E_1$.

To demonstrate this, we consider in the next section also the model bare density of states where, besides the symmetric smooth part $\rho_0(E)$, the bare DOS has near $\mu_{n+1}$ a narrow Lorentz peak with the width $\Gamma$,

$$\rho(E) = \rho_0(E) + \frac{h\Gamma}{(E - E_1)^2 + \Gamma^2}.$$  

(21)

One can see from Figure 4 that the Lorentz peak is considerably enhanced and narrowed by hybridization effects. Such an electronic structure is favorable for ferromagnetism since a part of the spin up peak is below the Fermi level which is in a local minimum.

5 Numerical calculation results

In the mean-field approximation, the total energy of the magnetic state is always lower than that of non-magnetic Kondo state,

$$\mathcal{E} - \mathcal{E}_{\text{non-mag}} = -J_0\bar{S}^2.$$  

(22)
Fig. 4. The partial spin-up (upper half) and spin-down (lower half) densities of states for the semielliptic bare band with the Lorentz peak. The vertical line is the chemical potential.

(see Appendix). Thus the formation of the state of a Kondo ferromagnet is energetically favorable. For the solutions with small moments the energy gain is smaller than for the half-metallic state, and the latter dominates provided that the corresponding solution does exist.

The Kondo ferromagnetic state energy should be also compared with the energy of the usual (Heisenberg) ferromagnetic state with the Kondo effect being suppressed ($W=0$, $\bar{S}=1/2$). The latter state becomes energetically favorable at rather large

$$j > j_c = 1/\left(1/4 - \bar{S}^2\right).$$  \hspace{1cm} (23)

At the critical point, a first-order magnetic transition should take place. Since the corresponding $j$ values are large, we will not show them on the plots below. We also do not discuss the phase boundaries corresponding to the left-hand inequality in (7) (for the cases considered below, this inequality starts to work and the HFM solution disappears nearly at the same values, $j > 5$).

The universal functions $L(\bar{S}, n)$, $P(\bar{S}, n)$, $M(n)$ and $Q(n)$, determining the magnetic solutions, depend on a bare density of states only and can be calculated for concrete lattices.

For simple lattices with a symmetric bare DOS, the non-saturated solution can exist only for $n < 1/2$ (where $\rho_{n+1} < \rho_n$). In particular, for the semielliptic bare band with

$$\rho_0(E) = \frac{4}{\pi D^2} \sqrt{D^2 - (2E - D)^2}$$

at $J_0 \to 0$ ferromagnetism disappears for $n > 0.5$, and saturated ferromagnetic solution occurs for $n < 0.42$. One can see from Figure 5 that for a given $n$ the value of $j$ depends very weakly on the moment and changes in a rather narrow interval. This interval reaches zero for $0.5 > n > 0.42$ where only the non-saturated solution exists at $j \to 0$. At the same time, the HFM solution at $n > 0.42$ can be restored by rather small $j$ (Fig. 6).

For the square lattice in the nearest-neighbor approximation (where bare DOS has a logarithmic singularity at the band centre) the HMF solution exists at $n < 0.5$. It is instructive to trace the influence of DOS singularity movement on the phase diagram in the case of square lattice with account of nearest and next-nearest transfer integrals, $t$ and $t'$. Figure 7 demonstrates that the ferromagnetic region grows for $t' > 0$ (the singularity is shifted to the band top) and diminishes for $t' < 0$ (the singularity is shifted to the band bottom). However, the region of the non-saturated solution never goes beyond the region of the HMF state.

For the simple cubic lattice (a more weak) Van Hove singularity in bare DOS (see Fig. 1) favours existence of saturated HFM solution, and the corresponding critical concentration at $j = 0$ increases up to 0.5 (Fig. 8). Thus the non-saturated state is again not energetically favorable.

The non-saturated solution for the bare DOS with a peak (21) is shown in Figure 9. One can see that

Fig. 5. The magnetization plots for the semielliptic bare band according to equation (13) for $n = 0.3, 0.35, 0.4, 0.45$ (from above to below).

Fig. 6. The surface plot of the non-saturated solution for the semielliptic bare band according to equation (13) (the left-hand sheet). The HFM solution exists above the right-hand sheet corresponding to the right-hand inequality equation (7).
small-moment magnetism occurs in a rather wide region near the $n$ values where $\mu_{n+1} = E_1$. Note that the HMF state does not exist in this concentration region, at least at small $j$. This case is most interesting from the point of view of analyzing experimental data on the ferromagnetic Kondo systems (see introduction).

6 Conclusions

We have demonstrated that the pseudofermion ferromagnetism in the Kondo lattices is a complicated phenomenon which has features of both itinerant electron and localized moment magnets. Under certain conditions, magnetic instability can occur at very small $J$ (even in comparison with $T_K$), which is characteristic for the Heisenberg systems. On the other hand, magnetic ordering is highly sensitive to electronic structure, as well as for itinerant systems. We have presented a rather simple description in terms of the ratio $j \sim J_0/T_K$ and universal functions that do not include the $s$-$f$ exchange parameter $I$ (or effective hybridization), but depend only on bare electron DOS $\rho(E)$.

The Kondo ferromagnetism has a number of peculiarities in comparison with the Stoner picture for usual itinerant systems. In particular, the dependence of ferromagnetism criterion on the bare density of states turns out to be different and more complicated. The reason is that $\sigma$-dependence of the effective hybridization plays a crucial role for this criterion.

Owing to hybridization character of spectrum and combined (electron-pseudo fermion) origin of the Fermi surface in the Kondo state, ferromagnetism is determined mainly by $\rho(\mu_{n+1})$ rather than by $\rho(\mu_n)$.

The hybridization form of the electron spectrum (presence of DOS peaks) in Kondo lattices is confirmed by numerous experimental investigations: direct optical data [24], observations of large electron masses in de Haas-van Alphen effect measurements, etc. Sometimes, intermediate valence (IV) and Kondo regime cannot be clearly distinguished in magnetism formation since $f$-states play anyway an important role in the electron structure near the Fermi level. The presence of “real” hybridization between $s$, $d$ and $f$-states in IV systems can induce bare DOS peak which, in turn, will influence pseudofermion ferromagnetism. A possible example is ferromagnetic CeRh$_3$B$_2$ with high Curie temperature and small saturation moment. However, neutron scattering analysis for CeRh$_3$B$_2$ revealed no magnetization on the rhodium and boron sites, so that ferromagnetism originates from the ordering of Ce local moments (and not, as has been claimed earlier, from itinerant magnetism in the Rh 4$d$ band) [25,26].

An unsolved problem is investigation of fluctuation effects beyond the mean-field approximation. In particular, they may destabilize ferromagnetism at small $j$. Simple spin-wave corrections discussed in reference [16] yield only formally small contributions to the ground state magnetization of order of $j \ln j$ (which are absent in the
HMF state). A more consistent consideration of fluctuations can be performed by using the slave-boson approach and the 1/N expansion within the periodic Anderson or Coqblin-Schrieffer model [27,28]. An interesting question is the role of fluctuation effects at finite temperatures, which should be even more important than in the ground state (as well as in usual itinerant magnets [29]).

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Appendix: Mean-field approximation in the pseudofermion representation

Making the saddle-point approximation for the path integral describing the spin-fermion interacting system [17] we reduce the Hamiltonian of the s-f model to the effective hybridization model (4). After the minimization for this Hamiltonian we obtain the equations for $W$, the chemical potential $\mu$ and magnetization $S$

$$n^f_\sigma = \frac{1}{2} \sum_k \left[ (1 - \cos \Theta_{k\sigma}) n^0_{k\sigma} + (1 + \cos \Theta_{k\sigma}) n^\beta_{k\sigma} \right],$$

$$n = \frac{1}{2} \sum_k \left[ (1 + \cos \Theta_{k\sigma}) n^0_{k\sigma} + (1 - \cos \Theta_{k\sigma}) n^\beta_{k\sigma} \right],$$

$$1 = -2I \sum_k \left( n^\beta_{k\sigma} - n^0_{k\sigma} \right) / E_{k\sigma}. \tag{A.9}$$

Then equations (A.1)–(A.3) take the form

$$n^f_\sigma = \frac{1}{2} \sum_k \left[ (1 - \cos \Theta_{k\sigma}) n^0_{k\sigma} + (1 + \cos \Theta_{k\sigma}) n^\beta_{k\sigma} \right],$$

$$n = \frac{1}{2} \sum_k \left[ (1 + \cos \Theta_{k\sigma}) n^0_{k\sigma} + (1 - \cos \Theta_{k\sigma}) n^\beta_{k\sigma} \right],$$

$$1 = -2I \sum_k \left( n^\beta_{k\sigma} - n^0_{k\sigma} \right) / E_{k\sigma}. \tag{A.7}$$

At small $|V_\sigma|, |W_\sigma|$ and $T = 0$ we have

$$\cos \Theta_{k\sigma} \simeq \text{sign} (t_k - \mu - W_\sigma), \tag{A.10}$$

so that equations (A.7) and (A.8) are further simplified.

The edges of the hybridization gaps in spin subbands are given by

$$E^\alpha_{k\sigma} > W_\sigma + V^2_\sigma / \mu, \quad E^\beta_{k\sigma} < W_\sigma - V^2_\sigma / (W - \mu). \tag{A.11}$$

Defining the function $\mu(n)$ by

$$n = 2 \int_0^{\mu(n)} \rho(E) \, dE, \tag{A.12}$$

equation (A.8) takes the form $\mu(n) = \mu$, and equations (A.7) and (A.9) yield at $W_\sigma > V^2_\sigma / (D - \mu)$

$$\lambda_\sigma \equiv V^2_\sigma / W_\sigma = \mu (n + 2n^f_\sigma) - \mu(n), \tag{A.13}$$

$$1 = -2I \int_0^{\mu + \lambda_\sigma} \frac{\rho(E)}{(E - \mu - W_\sigma)^2 + 4V^2_\sigma}^{1/2} \, dE. \tag{A.14}$$

In the leading approximation $V_\sigma$ does not depend on $\sigma$ and we have

$$|V_\sigma| \sim (DT_K)^{1/2}, \quad T_K = D \exp \frac{1}{2I \rho(\mu)}. \tag{A.15}$$

$$W \simeq V^2 / [\mu(n+1) - \mu] \sim T_K. \tag{A.16}$$

For $\rho(E) = \text{const}$, the calculations can be performed more accurately to obtain

$$|V_\sigma|^2 = \mu T_K / 2, \quad W_0 = \mu \exp \frac{1}{2I \rho} = \frac{nD}{2} \exp \frac{1}{2I \rho}. \tag{A.17}$$

To take into account spin polarization one has to calculate the integral in (A.14) to next-order terms in $1 / \ln |V_\sigma|/V_0$ [15,16]. One gets at neglecting $W_\sigma$

$$\left( \frac{V_\sigma}{V_0} \right)^2 = \exp \left( \frac{1}{\rho} \int_0^{\mu(n+1)} \frac{\rho(E)}{E - \mu} \, dE \right). \tag{A.18}$$
Using (A.13) and (A.18) we obtain

\[
\frac{W_\sigma}{W_0} = \exp \left( \frac{1}{\rho} \int_{\mu(n+1)} \frac{\rho(E) - \rho(\mu)}{E - \mu} dE \right) \tag{A.19}
\]

which yields the self-consistent equation for magnetization (11).

In the same way, for the half-metallic state (6) with \( \sigma = (1 - n)/2 \) we get

\[
1 = -2I \int_0^D \frac{\rho(E)}{(E - \mu)^2 + 4V_1^2}^{1/2} dE
\]

\[
= -2I \int_0^{\mu(2n)} \frac{\rho(E)}{(E - \mu)^2 + 4V_1^2}^{1/2} dE, \tag{A.20}
\]

\[
\lambda_1 = \mu(2n) - \mu(n). \tag{A.21}
\]

The ground state energy of the Kondo state is given by

\[
\mathcal{E} = \Omega(\mu(n)) + J_0 S^2 + \mu n - W, \tag{A.22}
\]

where the second term is introduced to compensate the “double-counted” terms, \( \Omega(\mu(n)) = \langle H - \mu n \rangle \). In our approximation of small \( V_2^2/D \) we derive

\[
\mathcal{E} - \mathcal{E}_{\text{non-mag}} = J_0 S^2 + \sum_\sigma n_\sigma(W_\sigma - W_0) - W + W_0 = -J_0 S^2 \tag{A.23}
\]

(the dependence of effective hybridization \( V \) on \( \sigma \) does not influence the magnetic energy since the non-universal hybridization does not enter \( \mathcal{E} [15, 16] \)).

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