

EFFECTIVE INTERACTIONS IN THE PERIODIC ANDERSON MODEL IN THE REGIME OF MIXED VALENCY WITH STRONG CORRELATIONS

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For the periodic Anderson model in the strong correlation regime, we construct the effective Hamiltonian H_{eff} up to terms of the fourth order in the parameter V/U , where V is the hybridization interaction intensity and U is the intra-atom Coulomb repulsion strength. This Hamiltonian contains interactions inducing both magnetic ordering and Cooper instability under conditions of a mixed valency of rare-earth ions. Based on numerical calculations, we obtain information about the dependences of the effective interaction parameters on the distance between crystal lattice sites. We demonstrate that realizing exchange interactions corresponds to a strongly frustrated system of localized spin moments and facilitates the suppression of the antiferromagnetic order parameter with a possible transition to the state of a quantum spin liquid. It is essential that among the terms in H_{eff} inducing the transition to the superconductivity phase, there are terms resulting in the d -type symmetry of the superconductivity order parameter; such a symmetry is realized in many heavy-fermion compounds.

Keywords: periodic Anderson model, mixed valency, heavy fermion, effective Hamiltonian, superconductivity

1. Introduction

The periodic Anderson model (PAM) has been actively used for several decades in theoretical studies of unusual properties of intermetallides containing ions of rare-earth and actinide elements (see, e.g., [1]). Depending on relations between the model parameters (the position of the localized level E_f , the collectivized electron band width W , the hybridization interaction intensity V , and the intra-atom Coulomb repulsion strength U), qualitatively different types of the system ground state are realized [2]. If we introduce the dimensionless coupling constant of the exchange between spin moments of localized and collectivized electrons $g = 2V^2\rho_c(\mu)|E_f - \mu|^{-1}$ (where μ is the chemical potential and $\rho_c(\mu)$ is the density of conductivity electrons in the Fermi level) [3], then the state of intermediate valency is realized for $g > 1$, while the system for $g < 1$ is either in the Kondo heavy-fermion regime, where the electronic specific heat and magnetic susceptibility are anomalously high in the low-temperature domain, or in the magnetic phase, where the RKKI interaction suppresses the Kondo fluctuations.

Passing to the effective Hamiltonian H_{eff} is customary when studying the low-energy part of the spectrum of the PAM elementary excitations [4]–[6]. The purpose of such a passage is to obtain effective interactions responsible for creating a ground state of a particular type and for forming the spectrum of elementary excitations. For example, the exchange and s – f -exchange interactions are relevant when studying conditions for the appearance of the long-range magnetic order and magnon branches of the

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spectrum. As is known, these interactions can be obtained in the PAM effective Hamiltonian in terms of the second and fourth orders in the small parameter V/U [7], [8]. The procedure for constructing H_{eff} is based either on using the unitary transformation method [7]–[12] (unitary transformations do not change the energy spectrum of a Hamiltonian) or on using the operator form of the perturbation theory [13], [14]. The structure of the effective Hamiltonian we obtain also depends on the operator representation, i.e., on whether we use the Fermi operators of the second quantization or the Hubbard operators satisfying more involved commutation (or anticommutation) relations.

The relation $W \ll V \ll U$ between the model parameters was used to derive the PAM low-energy effective Hamiltonian in [10]. The authors obtained H_{eff} by, first, using a unitary transformation to diagonalize the one-ion part of the PAM written in the Hubbard operators representation, second, projecting the transformation result on the low-energy subspace of states separated from excited states by a value of the order U and, third, applying the inverse unitary transformation. The effective Hamiltonian thus obtained allowed studying the problem of the existence of pairwise bound states in the PAM. The effective Hamiltonian up to the fourth order in V/U was constructed in [9] by consecutively applying two unitary transformations excluding hybridization transitions in the first and third orders. The main feature of the approach there was that the PAM Hamiltonian was first projected on the lower Hubbard subband (i.e., on the Hilbert subspace of localized states that do not contain two electrons) and only then were hybridization processes occurring in the lower Hubbard subband excluded by unitary transformations.

The unitary transformations $H \longrightarrow \tilde{H} = e^S H e^{-S}$ in most cases are performed under the condition that the anti-Hermitian operator S is written in terms of a combination of Fermi operators. In the Kondo regime, this allows eliminating hybridization processes between two subgroups of electrons in the first order and obtaining the effective Hamiltonian that, in particular, describes the exchange coupling between spin moments of the indicated groups of electrons. But it is known that this approach fails when the localized level is situated inside the continuum of collectivized states and close to the Fermi level. As shown in [12], values of exchange integrals then diverge. Nevertheless, this regime is especially interesting both from the standpoint of explaining the magnetic properties of some rare-earth and actinide intermetals and from the standpoint of finding explicit forms of effective interactions responsible for forming the Cooper instability in a system of heavy fermions. Moreover, it seems relevant to construct an effective Hamiltonian in the intermediate valency regime, which describes antiferromagnetic interactions that essentially influence the formation of the superconductivity phase with the order parameter having the d -type symmetry. This paper is devoted to considering these problems.

The key ingredient of our method is to split the hybridization interaction operator into two terms in the atomic representation. The first term reflects processes resulting in mixing collectivized and localized electrons without changing the number of states called the pairs in the localized subsystem (the low-energy sector of the Hilbert space). The second term is responsible for hybridization processes with simultaneous pair creation or annihilation; it explicitly takes processes inducing transitions to the high-energy sector of the Hilbert space into account. Because the energy parameter U is large, we can take these processes into account perturbatively, thus obtaining an analytic expansion in powers of the small parameter (see the actual applicability conditions for the expansion below). As a result, we obtain an effective Hamiltonian describing not only exchange interactions but also interactions explicitly indicating a possibility of the Cooper instability and the creation of a superconductivity phase with developed antiferromagnetic fluctuations.

2. Unitary transformations of the Hamiltonian

Using the atomic representation and splitting the hybridization interaction operator into two terms, we write the PAM Hamiltonian in the form

$$H = H_0 + V_{01} + V_{12}, \quad (1)$$

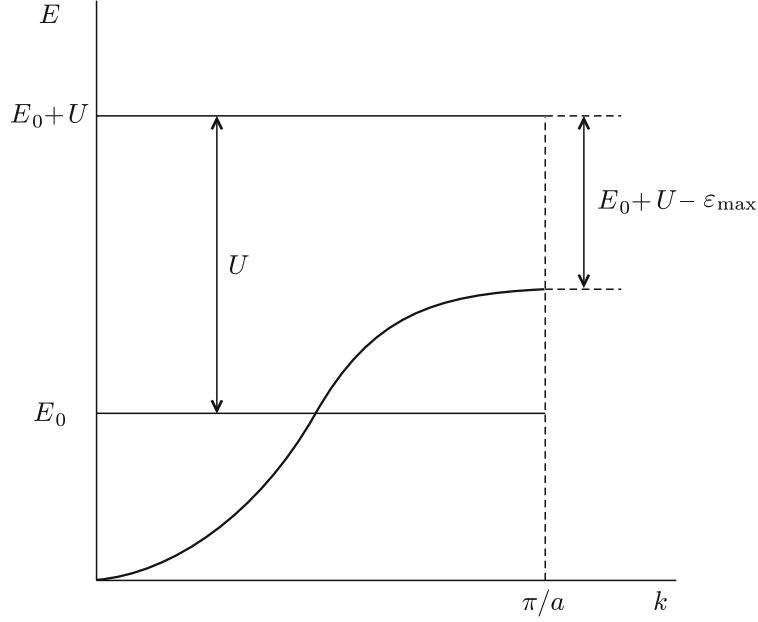


Fig. 1. The bare energetic structure of the periodic Anderson model.

where

$$\begin{aligned}
 H_0 &= \sum_{k\sigma} (\varepsilon_k - \mu) c_{k\sigma}^+ c_{k\sigma} + \sum_{f\sigma} (E_0 - \mu) X_f^{\sigma\sigma} + \sum_f (2E_0 - 2\mu + U) X_f^{22}, \\
 V_{01} &= \frac{1}{\sqrt{N}} \sum_{kf\sigma} (V_k e^{-ikf} c_{k\sigma}^+ X_f^{0\sigma} + V_k^* e^{ikf} X_f^{\sigma 0} c_{k\sigma}), \\
 V_{12} &= \frac{1}{\sqrt{N}} \sum_{kf\sigma} 2\sigma (V_k e^{-ikf} c_{k\sigma}^+ X_f^{\bar{\sigma}2} + V_k^* e^{ikf} X_f^{2\bar{\sigma}} c_{k\sigma}).
 \end{aligned} \tag{2}$$

Here, $c_{k\sigma}^+$ and $c_{k\sigma}$ are the creation and annihilation operators of the collectivized electron with the momentum k , spin moment projection $\sigma = \pm 1/2$, and energy ε_k . The Hubbard operators act in a subspace of localized states and are standardly defined as $X_f^{n,m} = |f, n\rangle\langle m, f|$. Each of the indices of the one-site localized state can take one of four values: $m, n \in \{0, \uparrow, \downarrow, 2\}$. The zero index indicates the one-site state without electrons. The vectors $|f, \uparrow\rangle$ and $|f, \downarrow\rangle$ correspond to the states with one electron that is localized at the site f and has the spin moment projection directed respectively along and against the quantization axis. These states have the bare energy E_0 . The vector $|f, 2\rangle$ describes states with two electrons localized at the site f (the so-called pairs). With the Coulomb interaction U taken into account, the bare energy of such a state is $2E_0 + U$. The diagonal Hubbard operator X_f^{nn} is a projection operator, while the nondiagonal operator X_f^{nm} with $n \neq m$ describes the transition from the one-site state $|f, m\rangle$ to the one-site state $|f, n\rangle$. We let V_k denote the Fourier transform of the hybridization interaction. It is important in what follows that the operator \widehat{V}_{12} , in contrast to the operator \widehat{V}_{01} , describes hybridization mixing processes with the simultaneous creation or annihilation of pair states from the Hilbert space high-energy sector.

For model parameters as in Fig. 1 with $|V_k| \ll E_0 + U - \varepsilon_{\max}$ (ε_{\max} is the maximum energy of the conductivity electron), we can take contributions of the operator \widehat{V}_{12} into account perturbatively. For this, we use the above inequality to construct the effective Hamiltonian, applying the sequence of unitary transformations.

At the first stage, we perform the unitary transformation $H \rightarrow \tilde{H} = e^S H e^{-S}$, choosing S to eliminate the operator V_{12} from the first-order term in the expansion of \tilde{H} . This requires that the operator equality

$$[S, H_0] = -V_{12} \quad (3)$$

determining S be satisfied. Simple calculations yield

$$S = -\frac{1}{\sqrt{N}} \sum_{kf\sigma} 2\sigma (\eta_k e^{-ikf} c_{k\sigma}^+ X_f^{\bar{\sigma}2} - \eta_k^* e^{ikf} X_f^{2\bar{\sigma}} c_{k\sigma}), \quad (4)$$

where the dimensionless parameter is

$$\eta_k = \frac{V_k}{U + E_0 - \varepsilon_k} \ll 1. \quad (5)$$

Expanding $\tilde{H} = e^S H e^{-S}$ in a series in η_k and restricting our consideration to terms up to and including the fourth order of smallness, we find that \tilde{H} is given by

$$\tilde{H} = H_0 + V_{01} + \left[S, \left(V_{01} + \frac{V_{12}}{2} \right) \right] + \left[S, \left[S, \left(\frac{V_{01}}{2} + \frac{V_{12}}{3} \right) \right] \right] + \left[S, \left[S, \left[S, \frac{V_{01}}{6} + \frac{V_{12}}{8} \right] \right] \right]. \quad (6)$$

We note that the obtained expression for \tilde{H} , starting with terms of the second order in η_k , again contains operators pertaining to the hybridization processes involving the high-energy sector of the Hilbert space. This means that such operators result in additional fourth-order contributions to the effective Hamiltonian. To calculate the corresponding operator expressions, we must use a multistage procedure for performing unitary transformations (see below).

Calculating the first commutators, we obtain the second-order contribution to \tilde{H}

$$\begin{aligned} \tilde{H}_{(2)} = & \sum_{fm\sigma} 2\sigma (t_{fm} X_f^{\sigma 0} X_m^{\bar{\sigma}2} + \text{H.c.}) + \frac{1}{N} \sum_{kpf} [\Delta_f(k, p) (c_{k\uparrow}^+ c_{p\downarrow}^+ - c_{k\downarrow}^+ c_{p\uparrow}^+) X_f^{02} + \text{H.c.}] + \\ & + \sum_{fm\sigma} t_{fm} X_f^{2\sigma} X_m^{\sigma 2} + \frac{1}{N} \sum_{qpf\sigma} A_f(q, p) (X_f^{\bar{\sigma}\sigma} c_{q\sigma}^+ c_{p\bar{\sigma}} - (X_f^{\bar{\sigma}\bar{\sigma}} + X_f^{22}) c_{q\sigma}^+ c_{p\sigma}). \end{aligned} \quad (7)$$

The operator terms in this expression describe four types of interactions. The first interaction type in the atomic representation is the set of quantum transitions between the lower and upper Hubbard subbands. The intensity of these transitions is determined by the matrix element

$$t_{fm} = \frac{1}{N} \sum_q \eta_q V_q^* e^{iq(f-m)}. \quad (8)$$

The second interaction type pertains to processes of creation or annihilation of pairs in the localized subsystem with the simultaneous annihilation or creation of a singlet pair of collectivized electrons with a not necessarily zero center-of-mass momentum. The intensity of such processes is described by the quantity

$$\Delta_f(k, p) = \eta_k V_p e^{-if(k+p)}. \quad (9)$$

The third interaction type is due to jumps of f electrons in the upper Hubbard subband with the matrix element t_{fm} . Finally, the last interaction type describes the exchange coupling and the Coulomb correlations between two electron subsystems. The intensity of these processes is proportional to

$$A_f(q, p) = \frac{1}{2} e^{-if(q-p)} [\eta_q V_p^* + \eta_p^* V_q]. \quad (10)$$

When writing contributions from higher-order commutators, we take into account that the final goal of our calculations is to construct the effective Hamiltonian H_{eff} up to and including terms of the fourth order of smallness. It is then important that the sector of the Hilbert space without pairs must be invariant under the action of H_{eff} . Introducing the operator of projection on this sector,

$$P = \prod_f (X_f^{00} + X_f^{\uparrow\uparrow} + X_f^{\downarrow\downarrow}), \quad (11)$$

we express this condition mathematically as

$$PH_{\text{eff}}P = PH_{\text{eff}} = H_{\text{eff}}P = H_{\text{eff}}. \quad (12)$$

Hence, the final contribution from the commutators of the third and fourth orders is determined only by terms projected to the sector without pairs. It is easy to see that because $P[S, [S, V_{12}]]P = 0$ and $P[S, [S, [S, V_{01}]]]P = 0$, the expressions for $\tilde{H}_{(3)}$ and $\tilde{H}_{(4)}$ determined by contributions from the remaining commutators are

$$\begin{aligned} \tilde{H}_{(3)} &= \frac{1}{2}P[S, [S, V_{01}]]P = \\ &= P \frac{1}{2\sqrt{N}} \sum_{f m k \sigma} [\eta_k t_{fm} e^{-ikf} (c_{k\bar{\sigma}}^+ X_f^{\sigma\bar{\sigma}} - c_{k\sigma}^+ X_f^{\bar{\sigma}\sigma}) X_m^{0\sigma} + \text{H.c.}] + \\ &+ P \frac{1}{2N^{3/2}} \sum_{k q p f \sigma} 2\sigma [\eta_q e^{-iqf} \Delta_f^*(k, p) X_f^{\bar{\sigma}0} c_{q\sigma}^+ (c_{k\downarrow} c_{p\uparrow} - c_{k\uparrow} c_{p\downarrow}) + \text{H.c.}], \end{aligned} \quad (13)$$

$$\begin{aligned} \tilde{H}_{(4)} &= \frac{1}{8}P[S, [S, [S, V_{12}]]]P = \\ &= P \frac{1}{8N} \sum_{k q f m \sigma} [\eta_q B_k^*(f, m) e^{-iqm} (c_{q\sigma}^+ X_m^{\bar{\sigma}\bar{\sigma}} - c_{q\bar{\sigma}}^+ X_m^{\sigma\sigma}) (c_{k\sigma} X_f^{\bar{\sigma}\bar{\sigma}} - c_{k\bar{\sigma}} X_f^{\sigma\sigma}) + \text{H.c.}] + \\ &+ P \frac{1}{4N^2} \sum_{p k q k_1 f \sigma} [\eta_{k_1} C_f^*(k, q, p) e^{-ik_1 f} c_{p\bar{\sigma}}^+ (c_{k_1\sigma}^+ X_f^{\bar{\sigma}\bar{\sigma}} - c_{k_1\bar{\sigma}}^+ X_f^{\sigma\sigma}) c_{k\bar{\sigma}} c_{q\sigma} + \text{H.c.}]. \end{aligned} \quad (14)$$

We define the functions in these relations as

$$\begin{aligned} B_k(f, m) &= 2\eta_k t_{fm} e^{-ikf} + \frac{2}{N} \sum_p \eta_p A_f(k, p) e^{-ipm}, \\ C_f(k, q, p) &= \eta_k A_f(q, p) e^{-ikf} + \eta_q A_f(k, p) e^{-iqf}. \end{aligned} \quad (15)$$

Collecting the obtained relations together, we obtain

$$\tilde{H} = H_0 + V_{01} + \tilde{H}_{(2)} + \tilde{H}_{(3)} + \tilde{H}_{(4)}. \quad (16)$$

It follows from expression (7) that the first two sums in the right-hand side of this equality describe processes resulting in changing the number of pairs in the system. Because these operators are of the second order of smallness, the processes of pair creation with their subsequent annihilation result in an additional interaction of the fourth order. To find the contributions of these processes, we perform the second unitary transformation, which does not change the operators $\tilde{H}_{(3)}$ and $\tilde{H}_{(4)}$ within the required accuracy. The desired effective Hamiltonian H_{eff} is then

$$H_{\text{eff}} = P e^{S_1} \tilde{H} e^{S_1} P. \quad (17)$$

We choose the operator S_1 determining the unitary transformation to exclude the second-order processes generating pairs from the expression $e^{S_1} \tilde{H} e^{S_1}$. We achieve this by choosing S_1 in the form

$$S_1 = \left\{ \frac{1}{N} \sum_{kpj} \left[\frac{\Delta_f(k, p)}{\varepsilon_k + \varepsilon_p - U - 2E_0} \right] (c_{k\uparrow}^+ c_{p\downarrow}^+ - c_{k\downarrow}^+ c_{p\uparrow}^+) X_f^{02} - \sum_{gm\sigma} 2\sigma \left(\frac{t_{gm}}{U} \right) X_g^{\sigma 0} X_m^{\bar{\sigma} 2} \right\} - \{\text{H.c.}\}. \quad (18)$$

After calculating the commutators and projecting to the Hilbert space sector without pairs, we obtain the effective Hamiltonian in its final form:

$$\begin{aligned} H_{\text{eff}} = & \sum_{k\sigma} (\varepsilon_k - \mu) c_{k\sigma}^+ c_{k\sigma} + \sum_{f\sigma} (E_0 - \mu) X_f^{\sigma\sigma} + \frac{1}{\sqrt{N}} \sum_{kf\sigma} [V_k e^{-ikf} c_{k\sigma}^+ X_f^{0\sigma} + \text{H.c.}] + \\ & + \frac{1}{N} \sum_{qpf\sigma} A_f(q, p) [c_{q\bar{\sigma}}^+ X_f^{\sigma\bar{\sigma}} - c_{q\sigma}^+ X_f^{\bar{\sigma}\bar{\sigma}}] c_{p\sigma} + \\ & + \frac{1}{2\sqrt{N}} \sum_{fmk\sigma} [\eta_k t_{fm} e^{-ikf} (c_{k\bar{\sigma}}^+ X_f^{\sigma\bar{\sigma}} - c_{k\sigma}^+ X_f^{\bar{\sigma}\bar{\sigma}}) X_m^{0\sigma} + \text{H.c.}] + \\ & + \frac{1}{2N^{3/2}} \sum_{kqpf} [\eta_q \Delta_f^*(k, p) e^{-iqf} (X_f^{l0} c_{q\uparrow}^+ - X_f^{l0} c_{q\downarrow}^+) (c_{k\downarrow} c_{p\uparrow} - c_{k\uparrow} c_{p\downarrow}) + \text{H.c.}] + \\ & + \frac{1}{N} \sum_{kqfms\sigma} \left[\frac{1}{8} \eta_q B_k^*(f, m) e^{-iqm} (c_{q\bar{\sigma}}^+ X_m^{\sigma\bar{\sigma}} - c_{q\sigma}^+ X_m^{\bar{\sigma}\bar{\sigma}}) (c_{k\bar{\sigma}} X_f^{\bar{\sigma}\sigma} - c_{k\sigma} X_f^{\bar{\sigma}\bar{\sigma}}) + \text{H.c.} \right] - \\ & - \frac{1}{N^2} \sum_{pkqk_1f\sigma} \left[\frac{1}{4} \eta_{k_1} C_f^*(k, q, p) e^{-ik_1f} c_{p\bar{\sigma}}^+ (c_{k_1\bar{\sigma}}^+ X_f^{\sigma\bar{\sigma}} - c_{k_1\sigma}^+ X_f^{\bar{\sigma}\bar{\sigma}}) c_{k\bar{\sigma}} c_{q\sigma} + \text{H.c.} \right] + \\ & + \frac{1}{N} \sum_{kpfm} \left\{ \left[\frac{\Delta_f(k, p)}{\varepsilon_k + \varepsilon_p - U - 2E_0} \right] t_{fm} (c_{k\uparrow}^+ c_{p\downarrow}^+ - c_{k\downarrow}^+ c_{p\uparrow}^+) (X_f^{0\downarrow} X_m^{0\uparrow} - X_f^{0\uparrow} X_m^{0\downarrow}) + \text{H.c.} \right\} + \\ & + \frac{1}{N^2} \sum_{kpfk_1p_1} \left[\frac{\Delta_f(k, p) \Delta_f^*(k_1, p_1)}{\varepsilon_k + \varepsilon_p - U - 2E_0} \right] X_f^{00} (c_{k\uparrow}^+ c_{p\downarrow}^+ - c_{k\downarrow}^+ c_{p\uparrow}^+) (c_{p_1\downarrow} c_{k_1\uparrow} - c_{p_1\uparrow} c_{k_1\downarrow}) + \\ & + \sum_{fm} J_{fm} \left(\vec{S}_f \vec{S}_m - \frac{1}{4} \hat{N}_f \hat{N}_m \right) + \sum_{\substack{fmg\sigma \\ (f \neq g)}} \left(\frac{t_{fm} t_{mg}}{U} \right) (X_f^{\sigma 0} X_m^{\bar{\sigma}\sigma} X_g^{0\bar{\sigma}} - X_f^{\sigma 0} X_m^{\bar{\sigma}\bar{\sigma}} X_g^{0\sigma}), \quad (19) \end{aligned}$$

where \vec{S}_f is the quasispin vector operator with the components

$$\begin{aligned} S_f^x &= \frac{S_f^+ + S_f^-}{2}, & S_f^y &= \frac{S_f^+ - S_f^-}{2i}, & S_f^z &= \frac{X_f^{\uparrow\uparrow} - X_f^{\downarrow\downarrow}}{2}, \\ S_f^+ &= X_f^{\uparrow\downarrow}, & S_f^- &= X_f^{\downarrow\uparrow}. \end{aligned}$$

The operators S_f^x , S_f^y , and S_f^z are quasispinorial because states without electrons are admissible at the site f . The operators S_f^x , S_f^y , and S_f^z therefore cannot be identified with spin operators although they rigorously satisfy the commutation relations specific for spin operators. This, for instance, follows from $(\vec{S}_f)^2 = (3/4) \hat{N}_f$, and only in the limiting case where exactly one electron is situated at each site f do the

quasispin operators become genuine spin operators. The operator $\hat{N}_f = \sum_{\sigma} X_f^{\sigma\sigma}$ is the number operator of localized electrons at the site f . The exchange interaction integral $J_{fm} = 2(t_{fm}t_{mf})/U$ has an origin analogous to that of the exchange coupling in the t - J model [15]. The projection operator is absent in the final expression for the effective Hamiltonian because the low-energy sector of the Hilbert space under investigation is invariant under the action of H_{eff} .

3. The hierarchy of effective interactions

We now describe the physical content of terms in PAM effective Hamiltonian (19). The first two terms of the Hamiltonian describe noninteracting subsystems of collectivized and localized electrons. For the localized electrons, we use the atomic representation with the Hilbert space not containing pairs, and we therefore call these electrons the Hubbard fermions in what follows. The third term describes the hybridization between two collectivized electrons and the Hubbard fermions.

In the second order in V_k , we have one term whose intensity is determined by the matrix element $A_f(q, p)$. It describes the scattering of conductivity electrons on localized f states. Some of these interactions reduce to the exchange s - f interaction, which, as is known, can induce singlet states of f and c electrons and can screen localized magnetic processes (the Kondo effect).

Interaction processes of the third order in V_k are described by two terms. The first is proportional to $\eta_k t_{fm}$ and describes hybridization processes between two groups of fermions correlated with the localized states. The second term describes the processes of annihilation or creation of a singlet pair in the collectivized electron subsystem with the simultaneous creation or annihilation of a combined singlet pair comprising the Hubbard fermion and the collectivized fermion. This interaction is obviously important for describing the superconductivity phase of rare earth intermetallics.

Effective Hamiltonian (19) contains six fourth-order terms. The term proportional to the matrix element $\eta_q B_k^*(f, m)$ describes the indirect exchange interaction of localized electrons via the collectivized states. The next term, which is proportional to $\eta_{k_1} C_f^*(k, q, p)$, describes a nonlocal pair interaction in the collectivized electrons subsystem with the bare scattering amplitude depending on the state of the Hubbard fermions. The last four terms in (19) arise as the result of the second unitary transformation. The first of them, which is proportional to $\Delta_f(k, p)t_{fm}$, describes processes of annihilation or creation of singlet pairs in the localized subsystem and the creation or annihilation of singlet pairs in the collectivized subsystem. This dynamical mixing of singlet pairs is also essential when describing the superconductivity phase. The next term, proportional to $\Delta_f(k, p)\Delta_f^*(k_1, p_1)$, describes the correlated dynamics of singlet pairs of the collectivized subsystem. The correlation means that the amplitude of the corresponding transitions decreases as the localized states are filled by Hubbard fermions. In particular, when the localized states are completely filled, such processes are totally damped. Finally, the last two terms describe the exchange interaction in the localized subsystem and also the three-center interactions (or the correlated jumps). As already mentioned, the origin of these terms is analogous to their origin in the derivation of the t - J model from the Hubbard model. The exchange interaction proportional to J_{fm} is important for describing the concurrence between the magnetic and superconductivity phases, as in the high-temperature superconductivity theory. It was recently shown that the three-center interactions essentially influence the domain of realization of the superconductivity phase with the $d_{x^2-y^2}$ -type symmetry of the order parameter. We should emphasize that while the last term is essential at a high level of filling the localized states, the preceding term is essential at a low level of filling the localized subsystem. This means that we must take both terms into account together when constructing the phase diagram expressing the concentration dependence of the critical temperature of the transition to the superconductivity phase, in particular.

We note that the dynamics of singlet pairs (becoming Cooper pairs at concrete momentum values) is governed by parameters of high orders in V_k in both the localized and collectivized subsystems in the

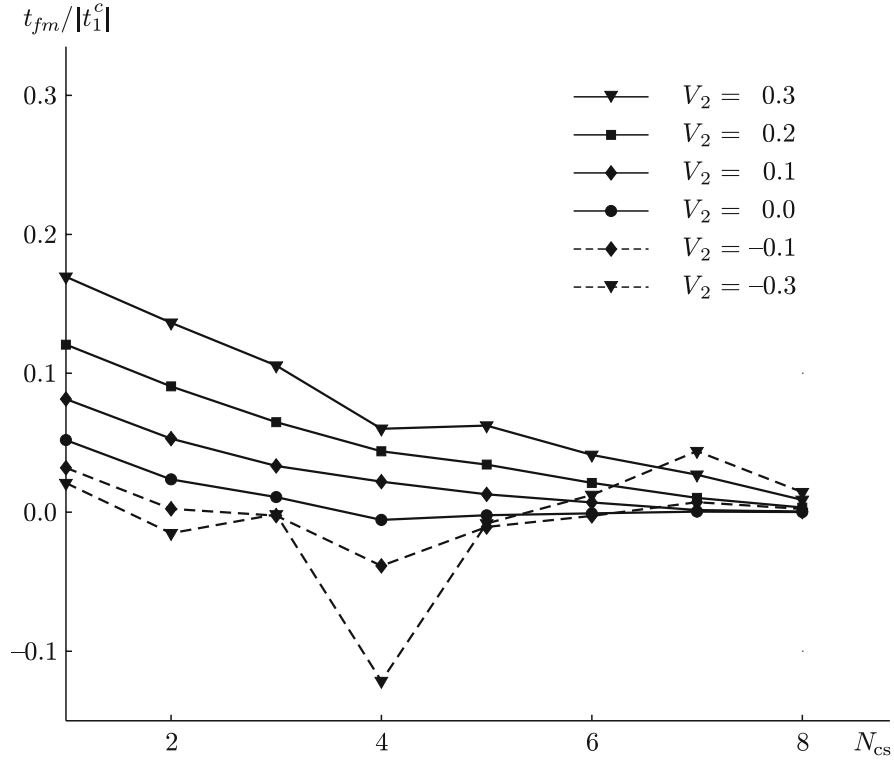


Fig. 2. The dependence of the effective jump integral on the coordinate sphere number at different values of the hybridization constant V_2 (see the PAM parameters in the text).

constructed effective Hamiltonian. This means that the simplest mean-field approximation already provides good accuracy when investigating the superconductivity phase and the concurrence between magnetic and superconductivity phases. But this set of questions goes beyond the scope of this paper, and the corresponding investigation results will be described in another paper. We confine ourselves here to addressing the important question about the magnitudes of exchange interactions in the framework of the obtained representations. The magnitudes of exchange parameters and their dependences on the distance are necessary for understanding the nature of the magnetically ordered phase.

The magnetic interaction in the localized subsystem is determined by two parameters. In addition to the next-to-last term with the parameter J_{fm} , the exchange interaction is formed by another term of the fourth order. Its intensity depends on B_k^* . After averaging over the states of the collectivized subsystem (as is customary in the RKKI theory), we obtain the expression describing the second indirect exchange interaction in the localized subsystem, which depends on the state of collectivized electrons:

$$H_{\text{exch}}^{(2)} = \sum_{fm} I_{fm} \left(\vec{S}_f \vec{S}_m + \frac{1}{4} \hat{N}_f \hat{N}_m \right), \quad (20)$$

where the exchange integral is

$$I_{fm} = \frac{1}{4N} \sum_k \eta_k B_k^*(f, m) e^{-ikm} n_k \quad (21)$$

and n_k is the distribution function of collectivized electrons. Adding the two contributions, we find that the exchange interaction in the localized subsystem of spin moments is described by the Hamiltonian

$$H_{\text{exch}} = \sum_{fm} \left\{ I_{fm} \left(\vec{S}_f \vec{S}_m + \frac{1}{4} \hat{N}_f \hat{N}_m \right) + J_{fm} \left(\vec{S}_f \vec{S}_m - \frac{1}{4} \hat{N}_f \hat{N}_m \right) \right\}. \quad (22)$$

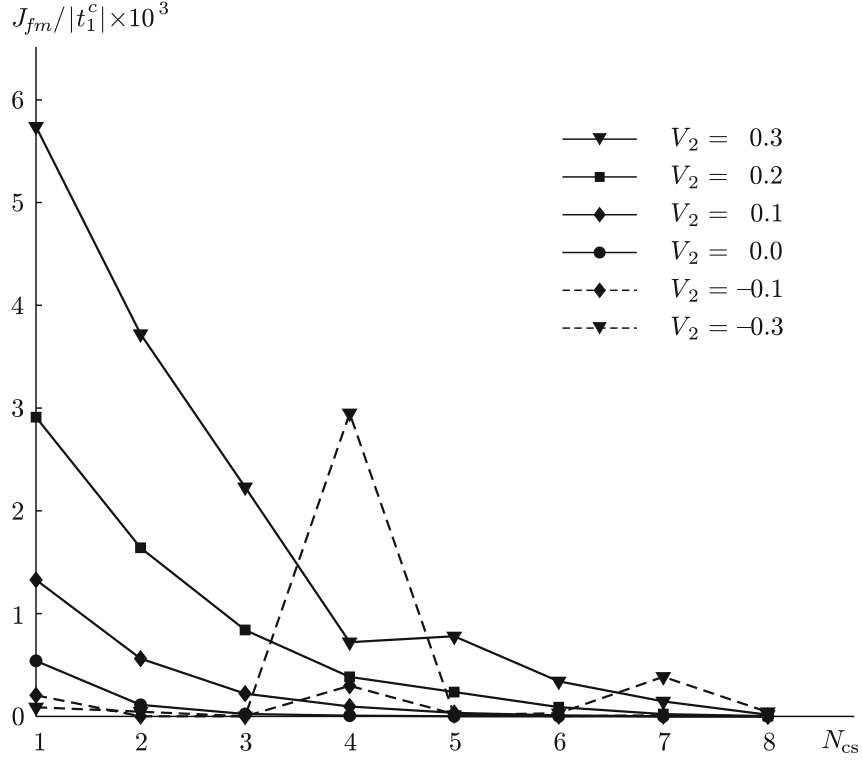


Fig. 3. The dependence of the super-exchange integral on the coordinate sphere number (see the PAM parameters in the text).

The quantities I_{fm} and J_{fm} are not independent and are expressed in terms of the parameters of the initial Anderson model; a comparative analysis of them therefore seems interesting for practical applications. For this, we use the results of numerical calculations of exchange integrals, paying special attention to the dependence of the exchange integrals on the distance between the lattice sites f and m . For convenience, we parameterize this distance by the coordinate sphere number N_{cs} . For definiteness, we assume that the ions of rare earth metals are placed at sites of the cubic lattice and the ions of the s and/or p elements forming the conductivity zone are placed at the centers of elementary cells. As follows from the expressions for I_{fm} and J_{fm} , the form of the c -electron dispersion ε_k affects the exchange integral values only slightly. We can therefore restrict ourselves to the strong-coupling limit when choosing ε_k :

$$\varepsilon_k = 2t_1^c(\cos k_x + \cos k_y + \cos k_z), \quad (23)$$

where t_1^c is the integral of the c -electron jump between the nearest ions of the s and p elements. At the same time, the dependence of V_k on the quasimomentum can be essential when calculating the values of the exchange integrals I_{fm} and J_{fm} . Taking this into account, we introduce two parameters V_1 and V_2 that we can use to express the intermixing of the orbitals of f and s or p ions. For V_k , we then have the expression

$$V_k = 8V_1 \cos \frac{k_x}{2} \cos \frac{k_y}{2} \cos \frac{k_z}{2} + 8V_2 \left(\cos \frac{3k_x}{2} \cos \frac{k_y}{2} \cos \frac{k_z}{2} + \cos \frac{k_x}{2} \cos \frac{3k_y}{2} \cos \frac{k_z}{2} + \cos \frac{k_x}{2} \cos \frac{k_y}{2} \cos \frac{3k_z}{2} \right). \quad (24)$$

In Figs. 2 and 3, we present the results of numerical calculations expressing the dependences of the effective f -electron jump integral t_{fm} and the super-exchange interaction parameter J_{fm} on the coordinate sphere

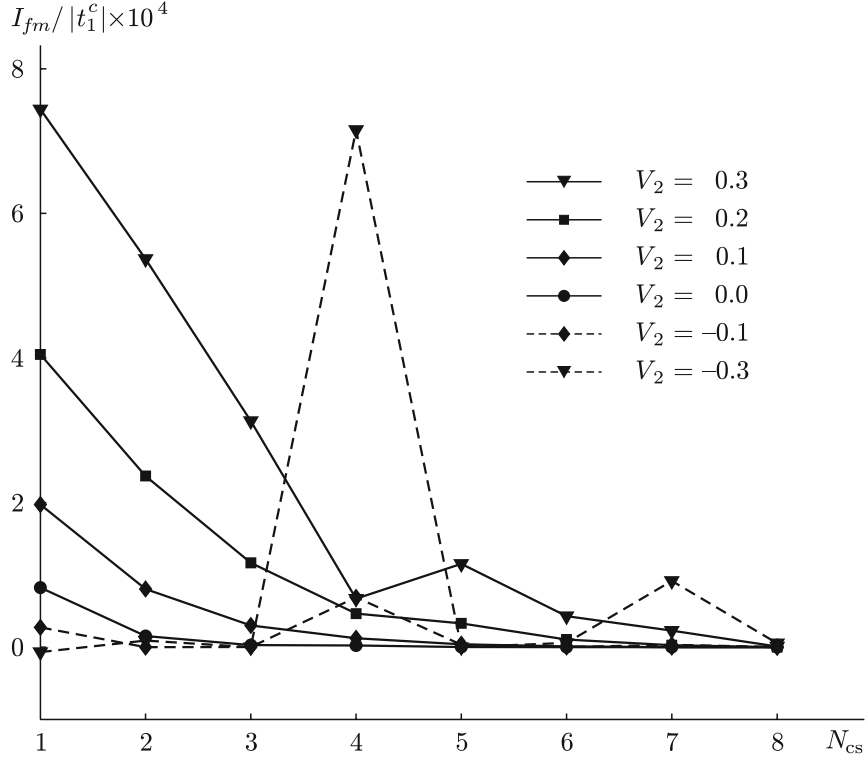


Fig. 4. The dependence of the integral of the indirect exchange interaction on the coordinate sphere number.

number N_{cs} at various values of the hybridization constant V_2 . The energy parameters are measured in units of $|t_1^c|$. The calculations were done with the PAM parameters $V_1 = 0.4|t_1^c|$, $E_0 = -2|t_1^c|$, and $U = 10|t_1^c|$. It follows from these figures that both t_{fm} and J_{fm} decrease monotonically for positive values of V_2 . The absolute value of the super-exchange interaction for nearest neighbors agrees well with the experimentally observed value of the Neel temperature in heavy-fermion systems: $T_N \sim 10$ K. An important property following from our calculations is that values of J_{fm} for the nearest and next-to-nearest neighbors differ by an inessential value on the order of 30%. Because both values are positive and the frustrated interaction effects are therefore essential, we can expect that the tendency to the magnetically ordered phase is damped and that a localized spin-moment system ground state of the spin-liquid type therefore forms. An interesting dependence occurs at $V_2 = -0.3|t_1^c|$, when the hybridization constant V_2 is close to $V_1 (= 0.4|t_1^c|)$ in absolute value but has the opposite sign. As shown in Fig. 3, the super-exchange interaction integral for the fourth coordinate sphere then substantially exceeds all other values of J_{fm} . This means that a subsystem of rare earth ions can then be split into eight cubic sublattices that do not interact with each other via the super-exchange mechanism. The sublattice parameter is then twice the parameter of the initial lattice. Inside each sublattice, the bonds are not frustrated, and $J_{fm} > 0$. This facilitates forming a long-range antiferromagnetic order. But the final spin configuration of the whole system then depends on other interaction types.

In Fig. 4, we present the results of calculating values of the indirect interaction exchange integral I_{fm} given by (21) at various distances between rare earth ions. For simplicity, the collectivized-electron distribution function n_k was approximated by the Fermi function with the bare energy spectrum for the collectivized electrons. The calculations were performed at the chemical potential $\mu = -2|t_1^c|$. The other PAM parameters were the same as in calculating I_{fm} . It can be seen from Fig. 4 that the indirect exchange

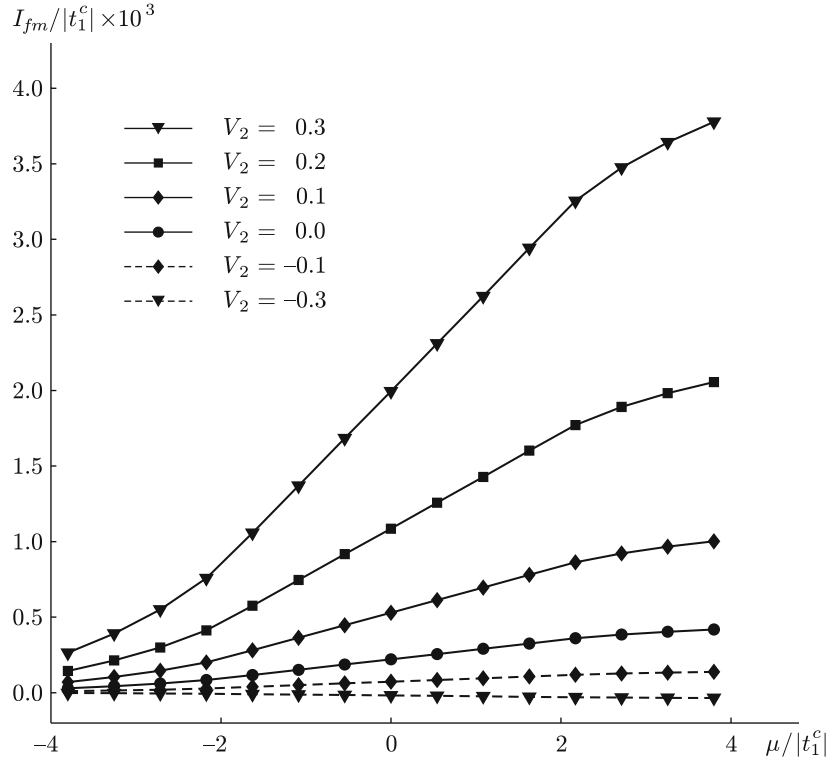


Fig. 5. The dependence of the integral of the indirect exchange interaction between nearest neighbors on the chemical potential at different values of the hybridization constant V_2 .

integral I_{fm} decreases as the coordinate sphere number increases. The absolute value of I_{fm} is then almost one order less than that for J_{fm} . Because the intensity of the indirect exchange interaction under consideration depends on the c -electron concentration, the value of I_{fm} can increase if the chemical potential increases. This can be seen in Fig. 5: the values of I_{fm} increase by almost an order as the conductivity zone fills. As a result, the coupling constants of the super-exchange and indirect exchange interactions can be comparable in order of magnitude for large concentrations of band electrons.

It follows from the above numerical analysis of two mechanisms of the exchange interaction (the indirect exchange and super-exchange) performed based on the obtained PAM effective Hamiltonian that concurrence between these two mechanisms of exchange interactions is absent in the whole range of the model parameters. The relative contribution of these two mechanisms in forming the system ground state depends both on the occupancy of localized orbitals and on the degree of filling of the conductivity zone.

In conclusion, we again mention that the key feature of our method for constructing the H_{eff} uses the smallness parameter determined by only those hybridization processes that involve high-energy states of the localized subsystem. Correspondingly, only these processes are excluded in the first and second order by using the unitary transformations. Hybridization processes then remain in the lower Hubbard subband. The common feature of the methods for obtaining the PAM H_{eff} mentioned in the introduction is the tendency to eliminate all the hybridization processes (both high-energy and low-energy ones). The reason that such a method is inapplicable to the mixed valency regime, as already mentioned, is that matrix elements of effective interactions obtained by integrating low-energy hybridization processes diverge.

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REFERENCES

1. E. Bauer et al., eds., *Phys. B*, **359–361** (2005); H. Harima et al., eds., *J. Magn. Magn. Mater.*, **310**, 169–944, 945–1882, 1883–2892 (2007).
2. Yu. A. Izyumov, N. I. Chashchin, and D. V. Alekseev, *Theory of Strongly Correlated Systems*, RKhD, Moscow (2006).
3. C. M. Varma, *Comments Solid State Phys.*, **11**, 221 (1985).
4. K. A. Kikoin et al., *Phys. Rev. B*, **59**, 15070–15084 (1999).
5. Y. Bang, “Mixed moment wave function for magnetic heavy fermion compounds,” arXiv:cond-mat/0206247v2 (2002).
6. C. Pépin, *Phys. Rev. Lett.*, **98**, 206401 (2007); arXiv:cond-mat/0610846v2 (2006).
7. J. R. Schrieffer and P. A. Wolff, *Phys. Rev.*, **149**, 491–492 (1966).
8. C. Lacroix and M. Cyrot, *Phys. Rev. B*, **20**, 1969–1976 (1979).
9. C. Proetto and A. López, *Phys. Rev. B*, **24**, 3031–3036 (1981).
10. D. F. Digor, P. Entel, and M. Marinaro, *Theor. Math. Phys.*, **127**, 664–675 (2001).
11. A. Hübsch and K. W. Becker, *Eur. Phys. J. B*, **52**, 345–353 (2006).
12. L.-J. Zhou and Q.-Q. Zheng, *J. Magn. Magn. Mater.*, **109**, 237–242 (1992).
13. S. V. Tyablikov, *Methods in the Quantum Theory of Magnetism* [in Russian], Nauka, Moscow (1965); English transl., Plenum, New York (1967).
14. P. Fulde, *Electron Correlations in Molecules and Solids* (Springer Ser. Solid-State Sci., Vol. 100), Springer, Berlin (1995).
15. Yu. A. Izyumov, *Sov. Phys. Uspekhi*, **40**, 521–523 (1997).