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Effect of Pressure on Antiferromagnetic and Superconducting Ordering in Systems with Heavy Fermions

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Abstract—Characteristics of the superconducting and antiferromagnetic phases of heavy-fermion intermetallides are described within a periodic Anderson model with allowance for the superexchange interaction between spin moments of the localized states. It is shown that an external pressure that changes the seed energy of an impurity level can rapidly destroy the long-range antiferromagnetic order. The development of the Cooper instability near such an order–disorder transition induces the experimentally observed state in which superconductivity coexists with the antiferromagnetic ordering.

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INTRODUCTION

In recent years, rare-earth intermetallides in which a series of phase transitions can be induced by applying an external pressure in zero magnetic field at low temperatures have been intensively studied. For example, the $CeRhIn_5$ compound at ambient pressure is an antiferromagnet with the Neel temperature $T_N = 3.8$ K [1]. As the pressure is increased slightly, the Neel temperature changes negligibly. In the vicinity of the critical pressure $P_c = 1.75$ GPa, however, the long-range antiferromagnetic order rapidly breaks down [2]. Data from nuclear quadrupole resonance [3] and neutron diffraction [4] show that at pressures below critical, a microscopically homogeneous phase emerges in which superconductivity (SC) coexists with antiferromagnetism (AFM).

Taking these experimental data into account, it seems reasonable to analyze the variation of the ground state of heavy-fermion (HF) systems under the action of an external pressure within the frequently used periodic Anderson model (PAM). This problem is solved in the context of an extended PAM that considers superexchange interaction in a subsystem of localized electrons. This approach is used because 4*f* Ce electrons participate in the formation of both the superconducting and antiferromagnetic orderings [3]. Note that the mixed phase in which SC is developed against the AFM background was observed earlier in an ensemble of itinerant electrons coupled by exchange interaction [5].

ANDERSON MODEL WITH SUPEREXCHANGE INTERACTION

We study the conditions for the emergence of the phase of coexisting SC and AFM in the HF intermetallides on the basis of the Hamiltonian

$$H_{\text{ef}} = \sum_{m\sigma}(\varepsilon_0 - \mu)c^{\dagger}_{m\sigma}c_{m\sigma} + \sum_{m\neq l\sigma} t_{ml}c^{\dagger}_{m\sigma}c_{l\sigma} + \sum_{m\sigma}(E_0 - \mu)X^{\sigma\sigma}_m + \sum_{ml\sigma}\left\{\left(V_{ml}c^{\dagger}_{m\sigma}X^{0\sigma}_l\right) + (\text{H.c.})\right\} + \frac{1}{2}\sum_{m\neq l} J_{ml}\left(\mathbf{S}_m\mathbf{S}_l - \frac{1}{4}N_mN_l\right). \quad (1)$$

The first and second terms of the Hamiltonian describe a subsystem of itinerant electrons with on-site energy ε_0 and matrix element t_{ml} of electron hoppings from site l to site m in the Wannier representation. The third term reflects the presence of localized states of 4*f* electrons with energy E_0 in the system. Hybridization processes with amplitude V_{ml} between two subsystems are described by the fourth term of the Hamiltonian. The last term takes into account the superexchange interaction; J_{ml} is the parameter of the exchange coupling between localized Hubbard fermions. This type of the superexchange interaction was established within the perturbation theory for the PAM with a large yet finite Coulomb repulsion parameter [6]. The scalar product of quasi-spin vector operators $\mathbf{S}_m$ and $\mathbf{S}_l$ is expressed via the Hubbard operators as

$$\mathbf{S}_m\mathbf{S}_l = \frac{1}{2} \times \left(X^{\uparrow\downarrow}_m X^{\downarrow\uparrow}_l + X^{\downarrow\uparrow}_m X^{\uparrow\downarrow}_l + \left(X^{\uparrow\uparrow}_m - X^{\downarrow\downarrow}_m\right)\left(X^{\uparrow\uparrow}_l - X^{\downarrow\downarrow}_l\right)/2\right).$$

The operator of the number of electrons localized on site m is $N_m = X_m^{\uparrow\uparrow} + X_m^{\downarrow\downarrow}$. The Hilbert subspace for the Hubbard operators of localized electrons is built on one state $|0\rangle$ without localized electrons on the site and two states $|\sigma\rangle$ with one localized electron with the spin moment projection $\sigma = \uparrow, \downarrow$; μ is the chemical potential of the system. The effect of the external pressure manifests itself through variations in energy E_0. This value grows with pressure, since cerium enters the $CeRhIn_5$ compound as a Ce^{3+} ion with a large resulting positive charge. Under the action of the pressure, the energy of the localized $4f$ Ce electron increases due to the Coulomb interaction with the effectively negative environment.

The problem is solved within the method of irreducible two-dimensional retarded Green's functions using the Zwanzig–Mori projection on an operator basis $\{X_f^{0\sigma}, Y_g^{0\sigma}, a_{f\sigma}, b_{g\sigma}, X_f^{\bar\sigma 0}, Y_g^{\bar\sigma 0}, a_{f\bar\sigma}^\dagger, b_{g\bar\sigma}^\dagger\}$ ($\bar\sigma = -\sigma$). The basis was selected with allowance for the existence of two antiferromagnetic sublattices. The normalization factors of the projection are $\alpha_\sigma = 1 - n_L/2 + \eta_\sigma R$ ($\eta_\sigma = \pm 1$ at $\sigma = \pm 1/2$, respectively), where the concentration of localized quasi-particles n_L and magnetization of the antiferromagnetic sublattice R are determined as

$$n_L = \langle X_f^{\uparrow\uparrow}\rangle + \langle X_f^{\downarrow\downarrow}\rangle, \quad R = \left(\langle X_f^{\uparrow\uparrow}\rangle - \langle X_f^{\downarrow\downarrow}\rangle\right)\Big/2. \quad (2)$$

The explicit structure of the numerators of normal $\left\langle\left\langle X_{p\sigma} \mid X_{p\sigma}^\dagger\right\rangle\right\rangle_\omega$ and anomalous $\left\langle\left\langle Y_{-p\bar\sigma} \mid X_{p\sigma}\right\rangle\right\rangle_\omega$ Green's functions is important in deriving the self-consistent equations. In the mean-field approximation for such functions taken with the opposite sign, we obtain

$$\begin{aligned}\alpha_\sigma S_{p\sigma}(\omega) &= \alpha_\sigma d_{3\bar\sigma}(p,-\omega) d_{4\sigma}(p,\omega)\\ &+ \alpha_\sigma\left(\frac{\Delta_p}{\alpha_{\bar\sigma}}\right)^2\left[(\omega-\xi_p)^2 - \Gamma_p^2\right] d_{3\sigma}(p,\omega),\end{aligned} \quad (3)$$

$$_\sigma A_{p\bar\sigma}(\ ) = \ _\sigma\ _{\bar\sigma}\quad {}_pQ_{p\bar\sigma}^{\pm}(\ )\quad {}_p^3R_{p\bar\sigma}(\ )\ , \quad (4)$$

respectively.

Here, we introduce the following denotations:

$$\begin{aligned}d_{3\sigma}(p,\omega) &= (\omega+E_\sigma)\left[(\omega+\xi_p)^2 - \Gamma_p^2\right]\\ &- \alpha_\sigma(\omega+\xi_p)\left(V_p^2 + W_p^2\right) + 2\alpha_\sigma\Gamma_p V_p W_p,\\ d_{4\sigma}(p,\omega) &= (\omega+E_{\bar\sigma}) d_{3\sigma}(p,\omega) + (\omega+E_\sigma) d_{3\bar\sigma}(p,\omega)\\ &- (\omega+E_\sigma)(\omega+E_{\bar\sigma})\left[(\omega+\xi_p)^2 - \Gamma_p^2\right]\\ &+ \alpha_\sigma\alpha_{\bar\sigma}\left(V_p^2 - W_p^2\right)^2,\\ f_3(p,\omega) &= 2(\omega+\xi_p) V_p W_p - \Gamma_p\left(V_p^2 + W_p^2\right),\end{aligned}$$

$$\begin{aligned}Q_{p\sigma}(\omega) &= \alpha_{\bar\sigma} f_3(p,\omega) f_3(p,-\omega)\\ &+ d_{3\sigma}(p,\omega) d_{3\sigma}(p,-\omega)/\alpha_{\bar\sigma},\\ R_{p\sigma}(\omega) &= \frac{1}{\alpha_{\bar\sigma}\alpha_\sigma^2}\left[(\omega+\xi_p)^2 - \Gamma_p^2\right]\left[(\omega-\xi_p)^2 - \Gamma_p^2\right].\end{aligned}$$

For the localized level energy renormalized by means of the existence of the exchange field of localized electrons and counted from the chemical potential, we introduce the denotation $E_\sigma = E_0 - \mu - 2J(n_L/2 + \eta_\sigma R)$. Symbols Γ_p and W_p denote the Fourier transforms of the integrals of hopping and hybridization between the sublattices, respectively. To characterize the intrasublattice hoppings and hybridization in the quasi-momentum space, we choose the denotations t_p and V_p, respectively. Fourier transform t_p now enters the definition $\xi_p = \varepsilon_0 + t_p - \mu$.

The quasi-average $\langle X_f^{\sigma\sigma}\rangle$ is determined from the equation ($f(x) = 1/(e^x + 1)$)

$$\begin{aligned}\langle X_f^{\sigma\sigma}\rangle &= \alpha_\sigma\left(\frac{1}{N/2}\right)\\ &\times \sum_{\substack{k\\ j=1..4}} \frac{S_{k\sigma}(-E_{jk}) f(-E_{jk}/T) - S_{k\sigma}(E_{jk}) f(E_{jk}/T)}{2E_{jk}\prod_{h\neq j}\left(E_{jk}^2 - E_{hk}^2\right)}.\end{aligned} \quad (5)$$

The concentration of itinerant quasi-particles is expressed as

$$n_c = \frac{1}{N/2}\sum_{k\sigma}\left\langle a_{k\sigma}^\dagger a_{k\sigma}\right\rangle, \quad (6)$$

where the quasi-average $\left\langle a_{k\sigma}^\dagger a_{k\sigma}\right\rangle$ is

$$\begin{aligned}&\langle a_{p\sigma}^\dagger a_{p\sigma}\rangle\\ &= \sum_{j=1..4} \frac{C_{p\sigma}(E_{jp}) f(E_{jp}/T) - C_{p\sigma}(-E_{jp}) f(-E_{jp}/T)}{2E_{jp}\prod_{h\neq j}\left(E_{jp}^2 - E_{hp}^2\right)}.\end{aligned} \quad (7)$$

In the last expression, we used the denotation

$$\begin{aligned}C_{p\sigma}(\omega) &= \left\{\left[(\omega-\xi_p)(\omega-E_\sigma) - \alpha_\sigma W_p^2\right](\omega - E_{\bar\sigma})\right.\\ &\left. - \alpha_{\bar\sigma} V_p^2(\omega - E_\sigma)\right\} d_{4\sigma}(p,\omega)\\ &- \Delta_p^2\left\{\left[(\omega-\xi_p)(\omega-E_{\bar\sigma}) - \alpha_{\bar\sigma}V_p^2\right]\left(\frac{d_{3\bar\sigma}(p,\omega)}{\alpha_\sigma^2}\right)\right.\\ &\left. - \frac{\Delta_p^2(\omega-\xi_p)}{(\alpha_\sigma\alpha_{\bar\sigma})^2}\left[(\omega+\xi_p)^2 - \Gamma_p^2\right]\right\}\\ &- \Delta_p^2\left\{\left[(\omega-\xi_p)(\omega-E_\sigma) - \alpha_\sigma W_p^2\right]\right.\\ &\left. \times\left(\frac{d_{3\sigma}(p,\omega)}{\alpha_{\bar\sigma}^2}\right) + 2f_3(p,\omega) V_p W_p\right\}.\end{aligned}$$

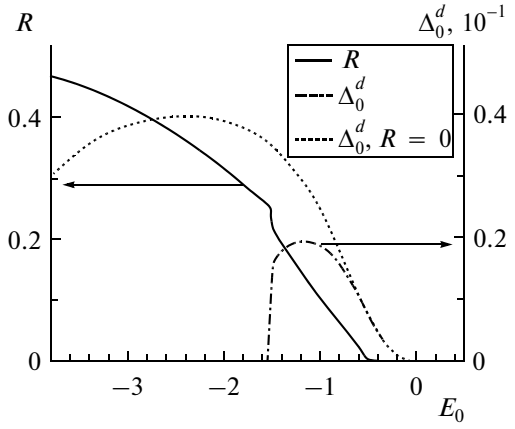

Fig. 1. Dependences of magnetization R (solid line) and amplitudes Δ_0^d of the superconducting order parameter calculated at $R = 0$ (dotted line) and self-consistently with regard to R (dash-dotted line) on energy E_0 of the localized level. The selected parameters of the model are $J = 0.2$, $V_0 = 0.6$, and $n_e = 1$.

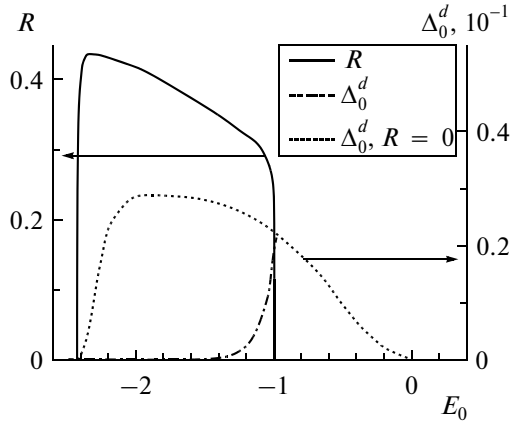

Fig. 2. Dependences of R and Δ_0^d on energy E_0 at $J = 0.2$, $V_0 = 0.6$, and $n_e = 1.2$.

The superconducting order parameter (SOP) Δ_p is defined as

$$\Delta_p = \frac{1}{N/2}\sum_q\left(\frac{1}{2}\right)\left[J_{p-q}\left\langle X_{q\uparrow}Y_{-q\downarrow}\right\rangle + J_{p+q}\left\langle Y_{q\uparrow}X_{-q\downarrow}\right\rangle\right]. \quad (8)$$

The use of (8) after substitution of the explicit expressions for the anomalous averages yields the integral equation for the SOP. Since the d-wave SC occurs in $CeRhIn_5$, the equation for the SOP amplitude Δ_0^d can be written as

$$\begin{aligned} 1 &= 2J\frac{1}{N/2}\sum_k\left[\sin\left(\frac{k_x b}{2}\right)\sin\left(\frac{k_y b}{2}\right)\right]^2 \\ &\times\sum_j\frac{-Q_k\left(E_{jk}\right)\tanh\left(E_{jk}/(2T)\right)}{2E_{jk}\prod_{h\neq j}\left(E_{jk}^2 - E_{hk}^2\right)} \\ &+ 8J(\Delta_0^d)^2\frac{1}{N/2}\sum_k\left[\sin\left(\frac{k_x b}{2}\right)\sin\left(\frac{k_y b}{2}\right)\right]^4 \\ &\times\sum_j\frac{-R_k\left(E_{jk}\right)\tanh\left(E_{jk}/(2T)\right)}{2E_{jk}\prod_{h\neq j}\left(E_{jk}^2 - E_{hk}^2\right)}. \end{aligned} \quad (9)$$

where $Q_k(\omega) = \sum_\sigma \alpha_\sigma Q_{k\bar{\sigma}}(\omega)$ and $R_k(\omega) = \sum_\sigma \alpha_\sigma R_{k\bar{\sigma}}(\omega)$.

RESULTS AND DISCUSSION

To study the effect of energy E_0 on the order parameters of the system (magnetization R and SOP Δ_p), it is sufficient to consider the low-temperature limit. Figure 1 shows the results from numerical calculations of self-consistent equations (2), (5), (7), and (9) for when the total electron concentration in the system $n_e = n_L + n_c = 1$. In this case, $J = 0.2$ and $V_0 = 0.6$. In the calculations, only hoppings between nearest neighbors with amplitude t_1 and on-site hybridization were taken into account. All of the energy quantities were normalized to the parameter $|t_1|$. It can be seen in Fig. 1 that magnetization R (solid line) decreases with increasing energy E_0, which can be attributed to the pressure growth. In the region where magnetization changes sharply, a superconducting gap with amplitude Δ_0^d (dash-dotted line) starts to form and a rather wide range of the energies occurs at which both the long-range antiferromagnetic order and superconducting pairing exist. Note that the formation of the antiferromagnetic order in the system led to a reduction in amplitude Δ_0^d. This is clearly demonstrated by the dotted curve that determines the dependence of Δ_0^d on energy E_0 at $R = 0$. At relatively low values of the total electron concentration, magnetization declines smoothly as E_0 rises. If the electron concentration is increased to $n_e = 1.2$, the dependence of magnetization on E_0 (pressure) becomes sharp. Such behavior (Fig. 2) corresponds to the experimental data for the $CeRhIn_5$ compound [3]. It can be seen that after attaining the critical energy value, magnetization drops sharply to zero. It is important that this happens near the maximum SOP amplitude point Δ_0^d. This indicates the competition between SC and AFM. It should be emphasized, however, that such a situation is not always observed. For example, at concentration $n_e = 1.5$, the occurrence of the antiferromagnetic order conversely induces Cooper instability (Fig. 3).

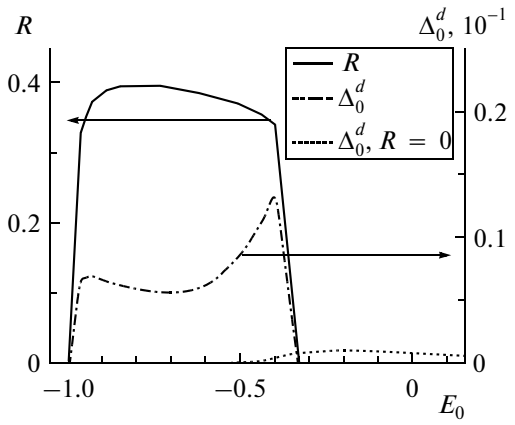

Fig. 3. Dependences of R and Δ_0^d on energy E_0 at $J = 0.2$, $V_0 = 0.6$, and $n_e = 1.5$.

CONCLUSIONS

The Anderson model, extended with allowance for the superexchange interaction in the subsystem of localized electrons describes the sharp suppression of the antiferromagnetic phase with increasing pressure and the formation of the phase in which antiferromagnetism and superconductivity coexist at the micron level. The phase diagram obtained by numerically solving self-consistent equations is in satisfactory agreement with the phase diagram based on the experimental data for $CeRhIn_5$.

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