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Anomalies in the Characteristics of Electronic Structure upon a Quantum Phase Transition to a State with Two Order Parameters and the Breaking of Time-Reversal Symmetry

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Abstract—Based on the periodic Anderson model, microscopic expressions for the Ginzburg–Landau expansion coefficients in a phase with superconducting and antiferromagnetic order parameters are obtained. Temperature dependences of the order parameters near the temperature of the transition to this phase are established. The emergence of anomalous properties upon the quantum phase transition to the phase with two order parameters is investigated. This transition is accompanied by drastic reconstruction of the density of states, reflected by the interplay between superconductivity and antiferromagnetism.

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INTRODUCTION

It is well known that Cooper pairing occurs between electronic states that transform one another during operations of time reversal. In antiferromagnetic materials, the symmetry relative to time reversal is broken. However, states coupled by the sequential application of time reversal and translation to the vector that relates ions from different sublattices in a magnetic unit cell have the same energy [1]. These states can participate in the formation of the Cooper instability of antiferromagnetic compounds.

Many cerium intermetallic compounds with heavy fermions are now known, including $CeIn_3$, $CeRhIn_5$, and $CePt_2In_7$ [2], in which the transition to a microscopically homogeneous phase with coexisting superconductivity and antiferromagnetism is induced at low temperatures and external pressures. It is of great interest to study the properties of such a phase with two order parameters and the breaking of time-reversal symmetry.

The Ginzburg–Landau (GL) phenomenological theory has been successfully used to describe new types of semiconductors. In [3], GL equations for superconductors with anisotropic order parameters were microscopically derived using Gor'kov's original technique. Microscopic GL equations were also derived for the *t*–*J* model in the slave-boson approximation [4].

Generalization of the GL theory to materials with a phase of coexisting superconductivity and antiferromagnetism has recently evoked special interest. A microscopic GL expansion in such a phase for the Hubbard and *t*–*J* models in a mean-field approximation was reported in [5, 6].

Based on the effective periodic Anderson model, in [7] we described the region of the coexistence of superconductivity and antiferromagnetism near the quantum critical point in the phase diagram of cerium intermetallic compounds. In [8], we showed that the effective electron mass is strongly renormalized and the Fermi surface is modified upon the transition through the quantum critical point.

In this work, we describe the microscopic derivation of GL equations for describing rare-earth intermetallic compounds with heavy fermions in a phase with antiferromagnetic and superconducting order parameters. We investigate features of the density of electronic states related to the quantum phase transition to such a phase upon varying the control parameters.

MODEL

Let us write the Hamiltonian of the effective periodic Anderson model, which allows for the exchange interaction in the subsystem of localized electrons:

$$H_{\text{eff}} = \sum_{m\sigma}\xi_c c^{\dagger}_{m\sigma}c_{m\sigma} + \sum_{ml\sigma}t_{ml}c^{\dagger}_{m\sigma}c_{l\sigma} + \sum_{m\sigma}\xi_L X^{\sigma\sigma}_m + \sum_{ml\sigma}\left(V_{ml}c^{\dagger}_{m\sigma}X^{0\sigma}_l + V^{*}_{ml}X^{\sigma 0}_l c_{m\sigma}\right) + \frac{1}{2}\sum_{ml}J_{ml}\left(\mathbf{S}_m\mathbf{S}_l - \frac{1}{4}N_m N_l\right). \quad (1)$$

The first and second terms of the Hamiltonian describe, in the Wannier representation, a subsystem of collective electrons with single-site energy ξ_c counted from the chemical potential and matrix element t_{ml} of electrons hopping from site l to site m. The localized electrons belonging to Wannier cell m are described in an atomic representation using Hubbard operators X_m^{ns}. The seed energy of a localized electron with regard to the chemical potential is denoted as ξ_L. Hybridization processes with amplitude V_{ml} between two subsystems are described by the fourth term of the Hamiltonian. The last term considers the exchange interaction in the localized subsystem. The magnitude of exchange interaction is specified by parameter J_{ml}, $\mathbf{S}_m$ is the quasi-spin vector operator, and N_m is the operator of the number of localized electrons on site m.

GINZBURG EXPANSION COEFFICIENTS IN THE PHASE OF COEXISTENCE

GL equations were derived in a generalized mean-field approximation using the Zwanzig–Mori projection technique for normal and anomalous Matsubara Green functions in a two-sublattice representation. Ignoring the magnetic field, we can write the system of GL equations in a site representation, leaving only the terms with superconducting d-symmetry order parameter Δ_f in the form

$$\begin{aligned}&\left[\alpha_s(T)+\beta_s\Delta_f^2+\gamma_1R_f^2\right]\Delta_f=0,\\&\left[\alpha_m(T)+\beta_mR_f^2+\gamma_2\Delta_f^2\right]R_f=0,\end{aligned}\qquad(2)$$

where R_f is sublattice magnetization and T is temperature. These equations are valid when temperature T_N of the onset of antiferromagnetic ordering and temperature T_s of the formation of superconductivity are similar.

The GL expansion coefficients are related to the microscopic parameters as

$$\begin{aligned}\alpha_s&=1-\frac{T}{N}\frac{4J}{F_0^2}\\&\times\sum_k\varphi_{d\mathbf{k}}^2\left[G_0^{FF}(-k)G_0^{FF}(k)+G_0^{GF}(-k)G_0^{GF}(k)\right],\end{aligned}\qquad(3)$$

$$\begin{aligned}\beta_s=\frac{T}{N}\frac{16J}{F_0^6}\sum_k\varphi_{d\mathbf{k}}^4\Big\{&\left[G_0^{FF}(-k)G_0^{FF}(k)\right.\\&\left.+G_0^{GF}(-k)G_0^{GF}(k)\right]^2+\left[G_0^{FF}(-k)G_0^{GF}(k)\right.\\&\left.+G_0^{GF}(-k)G_0^{FF}(k)\right]^2\Big\},\end{aligned}\qquad(4)$$

where $F_0=1-n_L/2$, n_L is the concentration of localized electrons, $k=(\mathbf{k}, i\omega_n)$ with Matsubara frequency ω_n, $\varphi_{d\mathbf{k}}$ is the basis function for d-type symmetry, and $G_0^{AB}(k)$ are the corresponding Green functions in the normal paramagnetic state. It is convenient to write the GL coefficients related to antiferromagnetic order as

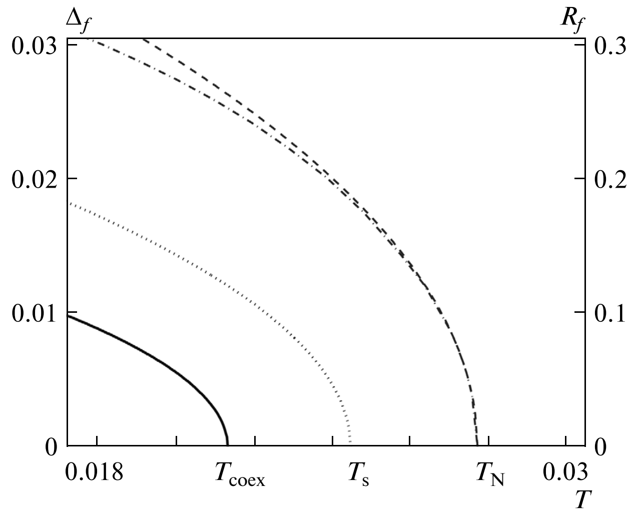

Fig. 1. Temperature dependence of antiferromagnetic order parameter R_f (dashed-and-dotted line) and superconducting order parameter Δ_f (solid line). The dashed line shows the approximate $R_f(T)$ dependence obtained using the Ginzburg–Landau theory; T_N is the Neel temperature. The dotted line shows the approximate $D_f(T)$ dependence, ignoring antiferromagnetism with temperature T_s of the onset of superconductivity and critical temperature T_{coex} of the mixed phase.

$$\begin{aligned}\alpha_m&=1-\frac{T}{N}\\&\times\sum_{\mathbf{k}\omega_n}\frac{(i\omega_n-\xi_L-F_0J_0/2)\left[(i\omega_n-\xi_{c\mathbf{k}})^2-\Gamma_\mathbf{k}^2\right]}{\prod\limits_{i=1,..,4}\left(i\omega_n-E_{i\mathbf{k}}^{(0)}\right)},\end{aligned}\qquad(5)$$

$$\begin{aligned}\beta_m=\frac{-T}{N}\sum_{\mathbf{k}\omega_n}\Bigg\{&\left(\frac{J_0}{2}\right)^2\left[(i\omega_n-\xi_{c\mathbf{k}})^2-\Gamma_\mathbf{k}^2\right]\\&-\left[J_0(i\omega_n-\xi_{c\mathbf{k}})-V_\mathbf{k}^2\right]V_\mathbf{k}^2\Bigg\}\\&\times\frac{(i\omega_n-\xi_L-F_0J_0/2)\left[(i\omega_n-\xi_{c\mathbf{k}})^2-\Gamma_\mathbf{k}^2\right]}{\prod\limits_{i=1,..,4}\left(i\omega_n-E_{i\mathbf{k}}^{(0)}\right)^2},\end{aligned}\qquad(6)$$

where $\xi_{c\mathbf{k}}$ is the energy of collective electrons in K-space with regard to hoppings inside the sublattice; $\Gamma_\mathbf{k}$ and $V_\mathbf{k}$ are the Fourier images integrals of hopping between sublattices and hybridization within the sublattice; and $E_{i\mathbf{k}}^{(0)}$ is the hybridization spectrum.

The presence of the terms with coefficients γ_1 and γ_2 in the microscopic GL equations (the analytical expressions for them are quite intricate) is related to the competition between superconductivity and antiferromagnetism, as has been experimentally observed in cerium intermetallic compounds with heavy fermions [9]. Figure 1 shows an example of the competition between superconductivity and antiferromagnetism.

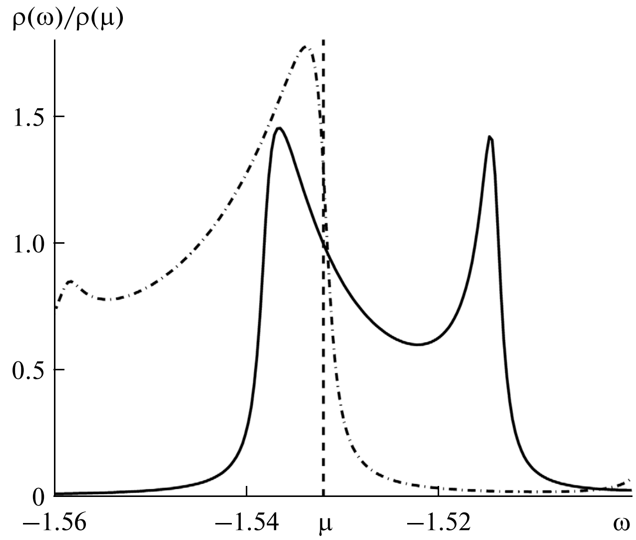

Fig. 2. Density of electronic states in the presence of antiferromagnetism (solid line) and in the paramagnetic state (dashed-and-dotted line) near energy $E_0 = -1.5$ for $J = 0.03$; $V = 0.3$. The vertical dashed line shows the level of chemical potential μ. The energies are given in units of $|t_1|$.

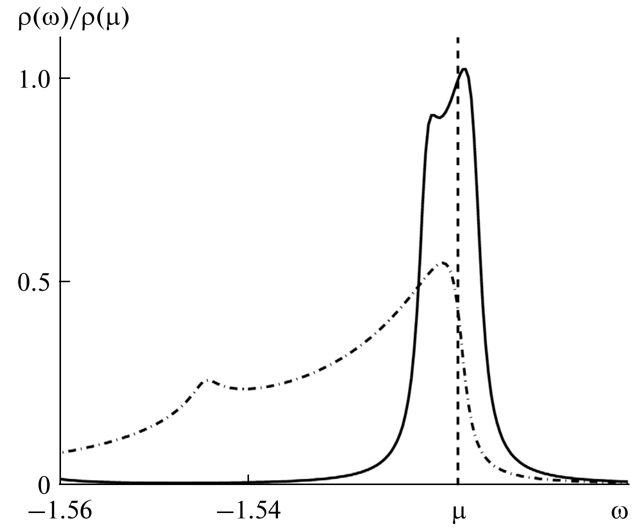

Fig. 3. Density of electronic states in the presence of antiferromagnetism (solid line) and in the paramagnetic state (dashed-and-dotted line) when $J = 0.01$.

The case $T_N > T_{cs}$ is considered. The dashed-and-dotted line shows the temperature dependence of antiferromagnetic order parameter $R_f(T)$, the values of which are plotted along the ordinate axis. The approximate $R_f(T)$ dependence obtained from the GL equations is shown by the dashed line. The dependences are consistent near T_N. The dotted line shows the dependence of the superconducting order parameter of *d*-type symmetry Δ_f in the GL theory with regard to the absence of the long-range antiferromagnetic order. When there is antiferromagnetism, the $\Delta_f(T)$ dependence has the shape shown by the solid line. It can be seen that in the antiferromagnetic state, the temperature of the onset of Cooper instability falls to T_{coex}, i.e., to the temperature of the transition to the phase of coexisting superconductivity and antiferromagnetism.

ANOMALOUS PROPERTIES UPON TRANSITIONING TO THE PHASE WITH TWO ORDER PARAMETERS

In the phase of coexisting superconductivity and antiferromagnetism, the superconducting order parameter is determined by two different contributions:

$$\Delta_p = \frac{1}{N/2}\sum_q \left(\frac{1}{2}\right)\left[J_{p-q}\left\langle X_{q\uparrow}Y_{-q\downarrow}\right\rangle + J_{p+q}\left\langle Y_{q\uparrow}X_{-q\downarrow}\right\rangle\right]. \quad (7)$$

The anomalous pairings in the first term are observed between electrons from different sublattices whose spin moments are co-directed with the magnetizations of the corresponding sublattices. The second type of Cooper pairings develop between electrons with spins directed opposite to the sublattice magnetizations. It is clear that the number of such electrons is much lower upon antiferromagnetic ordering. This indicates a simple qualitative mechanism of the suppression of superconductivity by antiferromagnetism, since both terms would make the same contribution in the absence of antiferromagnetic order.

When long-range antiferromagnetic order is induced and a transition to the mixed phase occurs, the density of electronic states changes considerably. This effect is illustrated in Fig. 2, where the dashed-and-dotted line shows the density of states for the paramagnetic case. The seed energy of the localized states is set at $E_0 = -1.5|t_1|$ and the parameters of interaction are $V = 0.3|t_1|$ and $J = 0.03|t_1|$, where t_1 is the amplitude of the hoppings of collective electrons between nearest sites ($t_1 < 0$). For cerium systems with heavy fermions, $|t_1|$ is estimated at 0.1–0.3 eV. The shift of the peak of density of states relative to energy E_0 corresponds to allowance for the mean-field renormalizations caused by exchange interaction. The vertical dashed line shows level of chemical potential μ.

When we consider the formation of antiferromagnetism, the density of states is transformed to the shape shown by the solid line in Fig. 2. The emergence of two peaks in the density of states is related to the loss of degeneracy for the energies of electrons from different antiferromagnetic sublattices. It can be seen that the onset of antiferromagnetism leads to a drop in the density of the state at the Fermi level. This is consistent with the intensity of Cooper pairings falling in the presence of antiferromagnetic ordering (Fig. 1).

Qualitatively different behavior is observed when the exchange interaction parameter is reduced to $J = 0.01|t_1|$. The exchange splitting of the energy level of localized electrons from different sublattices in the antiferromagnetic state is in this case slight, and the two peaks in the density of states merge (Fig. 3). At the onset of antiferromagnetism, the density of states at the Fermi level becomes larger than in the state without long-range magnetic order. At the onset of Cooper instability, antiferromagnetism will in this case facilitate superconductivity.

CONCLUSIONS

We obtained microscopic expressions for Ginzburg–Landau coefficients in a phase of coexisting superconductivity and antiferromagnetism for systems with heavy fermions described by the periodic Anderson model. It was established that the density of states is greatly renormalized with the occurrence of antiferromagnetism and the transition to the mixed phase. It was shown that antiferromagnetism can either suppress or facilitate Cooper pairings, depending on the nature of the variation in the density of states at the Fermi level.

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