PHYSICAL REVIEW B VOLUME 39, NUMBER 16 1 JUNE 1989

Superconductivity and spin-density waves in heavy-fermion systems

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(Received 24 October 1988)

Starting from a Kondo-lattice–type description, superconductivity and spin-density-wave coexistence is studied in the heavy-fermion systems. It is shown that the coexistence is energetically stable only in the presence of a supplementary Δ_Q superconducting order parameter connected to the $\langle a_{k,-\sigma}a_{-k-Q,\sigma}\rangle$-type average, where Q is the nesting wave vector.

The discovery of the heavy-fermion compounds was important because of the very unusual properties of the condensed phases of these materials. Of these properties, the existence of the anisotropic order parameters attracted the greatest attention. In the case of superconductivity, it is accepted that an unconventional type develops in some of these materials. In this connection Th-substituted UBe_{13} appears to be more and more important. The properties of this compound are briefly and in a very concise way reviewed by Sigrist and Rice,[1] where a qualitative explanation of many experimental facts are given, on the basis of a phenomenological theory and considering a transition between phases with different types of superconductivity.[2] On the same line Kumar and Wolfle[3] have investigated a simplified model with crossing s- and d-wave superconductivity. However, the presence of the inherent spin-density wave (SDW) is neglected in this analysis. In the case of related compounds, such as $(U_{1-x}Th_x)Pt_3$,[4] $U(Pt_{1-x}Pd_x)_3$,[5] and URu_2Si_2 (Ref. 6) the presence of SDW was already experimentally established. In the last case coexistence of a superconducting phase and SDW appears below 0.8 K.

The first proposal for the presence of SDW state in $(U_{1-x}Th_x)Be_{13}$ was given by Batlogg *et al.*,[7] starting from an ultrasonic study. The μSR experiments of Heffner, Cooke, and MacLaughlin[8] supported this proposal. The coexistence model of Machida and Kato[9] failed,[1] mainly because the second transition leads to an essential change in the superconductivity, as was shown by Rauchschwalbe *et al.*,[10] and even an increase in the superconducting condensation energy.

This is why the coexistence of superconductivity and SDW in heavy-fermion systems is a challenging problem, a comprehensive analysis of which is briefly presented here. Our study shows that in the case of heavy-fermion systems, the analyzed coexistence is stabilized only by a supplementary Δ_Q superconducting order parameter, which is connected to the $\langle a_{k,-\sigma}a_{-k-Q,\sigma}\rangle$-type average, where Q is the nesting wave vector. The analysis was made taking all the possible allowed combinations of different symmetry species of the superconductor and SDW order parameter.

For this we take into account a model Hamiltonian which describes a narrow heavy electron band starting from a Kondo lattice-type description

$$H_0 = -\tfrac{1}{2}\sum_{i,j,\sigma}(ta^\dagger_{i,\sigma}a_{j,\sigma}+\text{H.c.}) - \mu\sum_{i,\sigma}a^\dagger_{i,\sigma}a_{i,\sigma} + \tfrac{1}{2}\sum_{i,\sigma}Ua^\dagger_{i,\sigma}a_{i,\sigma}a^\dagger_{i,-\sigma}a_{i,-\sigma}\,, \quad (1)$$

where i and j denote the nearest-neighbor sites, the hopping energy t related to the bandwidth is given by $t=2T_K/z\pi$ (T_K and z being the Kondo temperature, and the number of the nearest-neighbor sites, respectively), μ is the chemical potential, and U is the renormalized, T_K-dependent on-site repulsion between the heavy electrons. Besides H_0 we take into account interactions between nearest-neighbor sites, which are phononic and magnetic in origin.

$$H_1 = -\tfrac{1}{2}\sum_{\{i_n\},\sigma,\sigma'}K(i_1,i_2,i_3,i_4;\sigma,\sigma')a^\dagger_{i_1,\sigma}a_{i_2,\sigma}a^\dagger_{i_3,\sigma'}a_{i_4,\sigma'}\,. \quad (2)$$

Such a term is necessary in order to describe the condensed phases in heavy-fermion systems, as was pointed out by Miyake, Matsuura, and Jichu,[11] and Czycholl and Doniach.[12] A comprehensive analysis of the K vertex is given in Ref. 13. For completeness, we consider all the possible allowed values of it.[13] The phononic term is taken into account in the $K(i,j,j,i;\sigma,\sigma')=V_1$ channel, and the spin-dependent terms by the $K(i,i,j,j;\sigma,\sigma') = V_2\delta_{-\sigma,\sigma'} - V_3\delta_{\sigma,\sigma'}$, $K(i,j,i,j;\sigma,-\sigma) = -V_4$ contributions. In order to describe the SDW phase,[14,15] we consider the nesting conditions to be satisfied at least along a fixed Q direction in the reciprocal space.[15] The order parameters describing the condensates are defined in the standard manner, and using the equation of motion method can be expressed as

$$\Delta^{(a)}(k) = \sum_i S_i(k)\Delta_i^{(a)}\,, \qquad \Delta_i^{(a)} = g_i^a\frac{1}{N}\sum_{k'}S_i(k')\Delta^{(a)}(k')\mathrm{I}_\mp^{(a)}(k')\,, \quad (3)$$

where $a=1,2$ represents the superconducting and the SDW phases, respectively. The 3D symmetry functions (here we analyze only the simple cubic case) are[14] $S_0(k)=1$,

$$S_1(k)=2(\cos ak_x+\cos ak_y+\cos ak_z)\,,$$

$$S_2(k)=\sqrt{6}(\cos ak_x-\cos ak_y)\,,$$

$$S_3(k)=\sqrt{2}(\cos ak_x+\cos ak_y-2\cos ak_z)\,,$$

$S_4(k)=\sin ak_x$, $S_5(k)=\sin ak_y$, and $S_6(k)=\sin ak_z$. (The extension to other crystal structures is straightforward.[15]) The effective coupling constants are the following:[13–15] $g_i^1=V_1+V_2$, $g_0^2=U+6(V_1+V_2+V_3)$, $g_i^2=V_3-V_4$; $i=1,2,3$, $g_i^2=V_3+V_4$; $i=4,5,6$.

The most important thing, neglected in Ref. 9, is that for the heavy-fermion Hamiltonian [Eqs. (1) and (2)], when both SDW and superconductivity pair amplitudes appear, a third pair amplitude inevitably occurs as a general requirement for self-consistency. This supplementary superconducting pairing is given by

$$\Delta_Q=g_Q\frac{1}{N}\sum_k\langle a_{k,-\sigma}a_{-k-Q,\sigma}\rangle\,, \tag{4}$$

which can be expressed as

$$\Delta_Q=g_Q\frac{1}{N}\sum_{k'}[\Delta_Q\mathrm{I}_+^{(1)}(k')+(\xi^2+\Delta^{(2)^2})^{1/2}\mathrm{I}_-^{(1)}(k')]\,, \tag{5}$$

where the effective coupling constant is $g_Q=6V_4-U$. The used kernel functions are

$$\mathrm{I}_\pm^{(1)}(k)=\frac{1}{4}\left[\frac{1}{\omega_+}\tanh\frac{\beta\omega_+}{2}\pm\frac{1}{\omega_-}\tanh\frac{\beta\omega_-}{2}\right],$$

$$\mathrm{I}_\mp^{(2)}(k)=\mathrm{I}_+^{(1)}(k)\pm\frac{\Delta_Q}{(\xi_k^2+\Delta^{(2)^2})^{1/2}}\mathrm{I}_-^{(1)}(k)\,, \tag{6}$$

with

$$\omega_\pm^2=\Delta^{(1)^2}+[(\xi_k^2+\Delta^{(2)^2})^{1/2}\pm\Delta_Q]^2,$$

and $\xi_k=-tS_1(k)-\mu$. In the case of pure phases ($\Delta_Q=0$, $g_i^1=0$, or $g_i^2=0$) we reobtain the description of the usual SDW (Refs. 14 and 15) or superconducting[16]

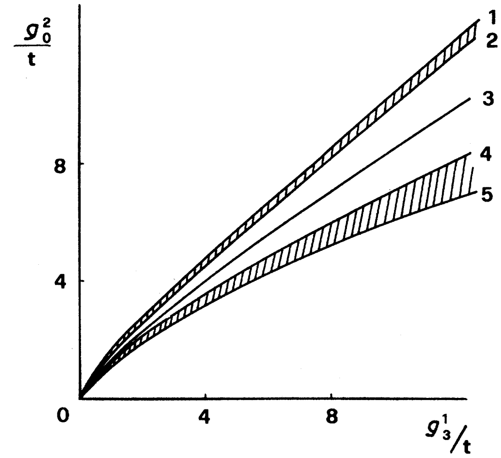

FIG. 1. Phase diagram in the $(g_0^2/t, g_3^1/t)$ plane. The pure superconducting (SDW) phase is situated between the g_3^1/t axis curve 5 (g_0^2/t axis curve 1). Line 3 represents the boundary between the simple superconducting and SDW phases when coexistence is not taken into account. Between curves 2 and 4 there is a metastable coexistence phase with $\Delta_Q=0$. The shaded area denotes the stable coexistence domain, i.e., $\Delta_Q\neq 0$, $\Delta^{(1)}\neq 0$, and $\Delta^{(2)}\neq 0$.

phases. We mention that the introduction of Δ_Q was made already some years ago[17] in another context, and was brought up to date for the high-T_c materials.[18] To give a realistic coexistence analysis, the free energy of an analyzed phase (F) was compared for every point of the phase diagram with the free energy of the paramagnetic phase (F_0), and with the free energy of the whole possible phases which can exist [i.e., allowed by the coupled order-parameter equations, Eqs. (3) and (5)] on the same point of the phase diagram. The obtained solution is stable energetically only if $\delta F<0$ ($\delta F=F-F_0$). The free energy can be expressed as $\delta F=\delta F_S+\delta F_{\mathrm{SDW}}+\delta F_Q+\delta F_{\mathrm{ln}}$, where the first three individual contributions are $\delta F_S=\sum_{i=1}^3\Delta_i^{(1)^2}/g_i^1$, $\delta F_{\mathrm{SDW}}=\sum_{i=0}^6\Delta_i^{(2)^2}/g_i^2$, $\delta F_Q=\Delta_Q^2/6V_4-U$. The last contribution can be written in the following way:

$$\delta F_{\mathrm{ln}}=-\frac{\beta^{-1}}{N}\sum_{k'}\left(\ln\cosh^3\frac{\beta\omega_+}{2}\cosh^3\frac{\beta\omega_-}{2}-\ln\cosh\frac{\beta\omega_+(\Delta^{(1)}=0)}{2}\cosh\frac{\beta\omega_-(\Delta^{(1)}=0)}{2}\cosh\frac{\beta\omega_+(\Delta^{(2)}=0)}{2}\right.$$
$$\left.-\ln\cosh\frac{\beta\omega_-(\Delta^{(2)}=0)}{2}\cosh\frac{\beta\omega_+(\Delta_Q=0)}{2}\cosh\frac{\beta\omega_-(\Delta_Q=0)}{2}\right),$$

which in the $T=0$ limit becomes

$$\delta F_{\mathrm{ln}}=-\frac{1}{N}\sum_{k'}\{\tfrac{3}{2}(\omega_++\omega_-)-\tfrac{1}{2}[\omega_+(\Delta^{(1)}=0)+\omega_-(\Delta^{(1)}=0)+\omega_+(\Delta^{(2)}=0)$$
$$+\omega_-(\Delta^{(2)}=0)+2(\xi_{k'}^2+\Delta^{(1)^2}+\Delta^{(2)^2})^{1/2}]\}\,.$$

The analysis of the phase diagram in the space of coupling constants revealed an energetically stable coexistence domain in the (g_3^1, g_0^2) plane, which has the form $\Delta_Q\neq 0$, $\Delta_3^{(1)}\neq 0$, and $\Delta_0^{(2)}\neq 0$ (d symmetry superconductor, and k independent SDW). This domain is stabilized by the $\Delta_Q\neq 0$ value. The other coexistence phases are metastable. The phase diagram is represented in Fig. 1.

This result shows that if an SDW phase will appear in a superconducting one, then this will imply the emergence of a Δ_Q phase. This last being a supplementary superconducting phase, its emergence explains the H_{c1} slope increase observed in $(U_{1-x}Th_x)Be_{12}$ (Ref. 10), and also the different specific-heat jump measured[19] for the two transitions.

As an interesting observation, we mention that the Δ_Q phase cannot appear alone (i.e., $\Delta^{(1)}=0, \Delta^{(2)}=0$). Indeed for the critical temperature of the Δ_Q phase (T_{cQ}) we obtain $\frac{1}{2} g_Q N(0) = \tanh \Omega / 2T_{cQ}$. From this it can be seen, that for $q_Q < \frac{1}{2} N(0)$ $T_{cQ}=0$ is obtained. As it is known, in the case of heavy-fermion systems $N(0)$ is very high. From the other hand, V_4 is usually a small[14,15] quantity; therefore $g_Q = 6V_4 - U$ cannot be greater than $\frac{1}{2} N(0)$. In fact, the $T=0$ phase diagram of the system does not contain an energetically stable $\Delta_Q \neq 0$ ($\Delta^{(1)}=0, \Delta^{(2)}=0$) phase.

The authors kindly acknowledge the hospitality of University of Frankfurt and Theoretische Physik, Eidgenössische Technische Hochschule Zürich-Hönggerberg. The authors also wish to thank M. Sigrist for providing his manuscript before publication.

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