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LETTER TO THE EDITOR

Stimulation of superconductivity by an antiferromagnetic ordering in heavy-fermion compounds

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Abstract. Using the high degenerate model we show that an antiferromagnetic ordering of localized moments in the coherent Kondo state stimulates superconductivity in heavy-fermion compounds. We find also that the antiferromagnetic moment per f-atom is anomalously small.

Many experimental investigations of heavy-fermion compounds such as UBe_{13}, UPt_3, URu_2Si_2 and $CeCu_2Si_2$ have shown that the superconductivity of these compounds is remarkable and is supposed to occur via an electron mechanism rather than a phonon one (see [1–5]). At temperatures below the Kondo temperature, T_K, these compounds are in the heavy-fermion ground state characterized by an enhanced electron mass on the Fermi surface (for example, $m^* \approx 200m_0$ for UPt_3 [6], $m^* \approx m_0$ for UBe_{13} [7]). At a lower temperature, T_N, these compounds undergo an antiferromagnetic transition. This antiferromagnetic state is also unusual since in this state the antiferromagnetic moments of U-atoms are anomalously small (for example, $\mu \approx 0.02\mu_B$ for UPt_3 [8], $\mu \approx 0.04\mu_B$ for URu_2Si_2 [9, 10]). Then at a temperature $T_c \sim 0.1\ T_N$ these compounds become superconducting.

In the present letter we discuss the problem of an interplay between the Kondo effect, antiferromagnetism and superconductivity. For this purpose we use a new model based on the Coqblin–Schrieffer lattice Hamiltonian. In our previous paper [11] we have used the model to study magnetic properties of heavy-fermion compounds. It has been shown that the coherent Kondo state is unstable against an antiferromagnetic ordering of localized moments when the Fermi surface of the conduction band possesses nesting. Here we shall show that in the framework of our model at $T \ll T_N \ll T_K$ the antiferromagnetic state is characterized by a very small antiferromagnetic moment per f-atom. Kondo screening is the reason for this phenomena. Introducing an additional exchange interaction between conduction electrons and localized f-electrons, we study superconductivity in the framework of the mean-field theory. We find that the antiferromagnetic state stimulates superconductivity. What is more the superconductivity can arise only at $T_c < T_N$. It is the antiferromagnetic ordering that leads to superconductivity.

We study a system described by the Hamiltonian

$$H = \sum_{\sigma k} \epsilon_k c^+_{\sigma k} c_{\sigma k} - \frac{1}{N} \sum_{\sigma \eta i} \left(J f^+_{\sigma i} c_{\sigma i} c^+_{\eta i} f_{\eta i} + J_2 f^+_{\sigma i} c^+_{-\sigma i} c_{-\eta i} f_{\eta i} \right) + \frac{J_1}{N} \sum_i S^z_i s^z_i \tag{1}$$

where $c^+_{\sigma k}$ and $c_{\sigma k}$ are the creation and annihilation operators for conduction electrons with wave number k and spin quantum number σ. The spin quantum numbers σ and η run from $-j$ to j; $N = 2j+1$ is the spin degeneracy. $f^+_{\sigma i}$ and $f_{\sigma i}$ are the creation and annihilation operators for f-electrons localized at points R_i. The operators S^z_i and s^z_i of moments for f-electrons and c-electrons are given by

$$S^z_i = \frac{1}{N}\sum_\sigma \sigma f^+_{\sigma i} f_{\sigma i} \qquad s^z_i = \frac{1}{N}\sum_\sigma \sigma c^+_{\sigma i} c_{\sigma i}. \tag{2}$$

The constraints

$$\sum_\sigma f^+_{\sigma i} f_{\sigma i} = q_0 N \tag{3}$$

are imposed for each i. At $J_1 = J_2 = 0$, Hamiltonian (1) is equal to the Coqblin–Schrieffer Hamiltonian [12]. In the framework of the mean-field theory the exchange constant J_1 introduces the Ruderman–Kittel–Kasuya–Yoshida (RKKY)-interaction with the characteristic energy $\rho_0 J_1^2$ where ρ_0 is the density of states at the Fermi level for the conduction band ϵ_k. The exchange interaction characterized by the constant J_2 leads to superconductivity as will be shown below. Here we suppose that the constants J, J_1 and J_2 are positive.

Using the Hubbard–Stratonovich transformation and taking into account constraints (3), one can write the partition function of model (1) as path integrals over the Grassmann variables c^+, c, f^+, f and Bose variables b^*, b, ψ^*, ψ, Δ^*, Δ, λ:

$$Z = \int D(c^+ c f^+ f b^* b \psi^* \psi \Delta^* \Delta \lambda) \exp\left(-\int_0^\beta \mathrm{d}\tau \; L(\tau)\right)$$

$$\begin{aligned} L(\tau) = {} & \sum_{\sigma k} c^+_{\sigma k}(\partial_\tau + \epsilon_k - \mu) c_{\sigma k} + \sum_{\sigma i} f^+_{\sigma i}(\partial_\tau - \mu) f_{\sigma i} \\ & + \sum_i \bigg(\frac{N}{J} b^*_i b_i + N J_1 \psi^*_i \psi_i + \frac{N}{J_2}\Delta^*_i \Delta_i - J_1 \psi_i S^z_i + J_1 \psi^*_i s^z_i \\ & - \sum_\sigma (b^*_i f^+_{\sigma i} c_{\sigma i} + \Delta_i f^+_{\sigma i} c^+_{-\sigma i} + \mathrm{H.c.}) + \mathrm{i}\lambda_i \sum_\sigma (f^+_{\sigma i} f_{\sigma i} - q_0) \bigg) \end{aligned} \tag{4}$$

where μ is the chemical potential. In the high degeneracy limit $N \gg 1$ the integration over the Bose variables may be performed by using the saddle-point method. The structure of the ground state is determined by the relations of the constants J, J_1 and J_2 to each other, the Fermi surface and the space arrangement of the localized moments [11].

For simplicity we shall study the system with cubic symmetry in which the c- and f-sublattices coincide. At first we suppose that the total number of c- and f-electrons is equal to 1/2, that is $n_t = n_c + q_0 = 1/2$. If the exchange constant J is larger than J_1 and J_2, then at temperatures $T < T_K$ the uniform coherent Kondo state is formed ($b_i = b^*_i = b \neq 0$). This state is characterized by the effective hybridization parameter b between c- and f-electrons and the effective f-level energy $\epsilon_f = \mathrm{i}\lambda_i$ [13].

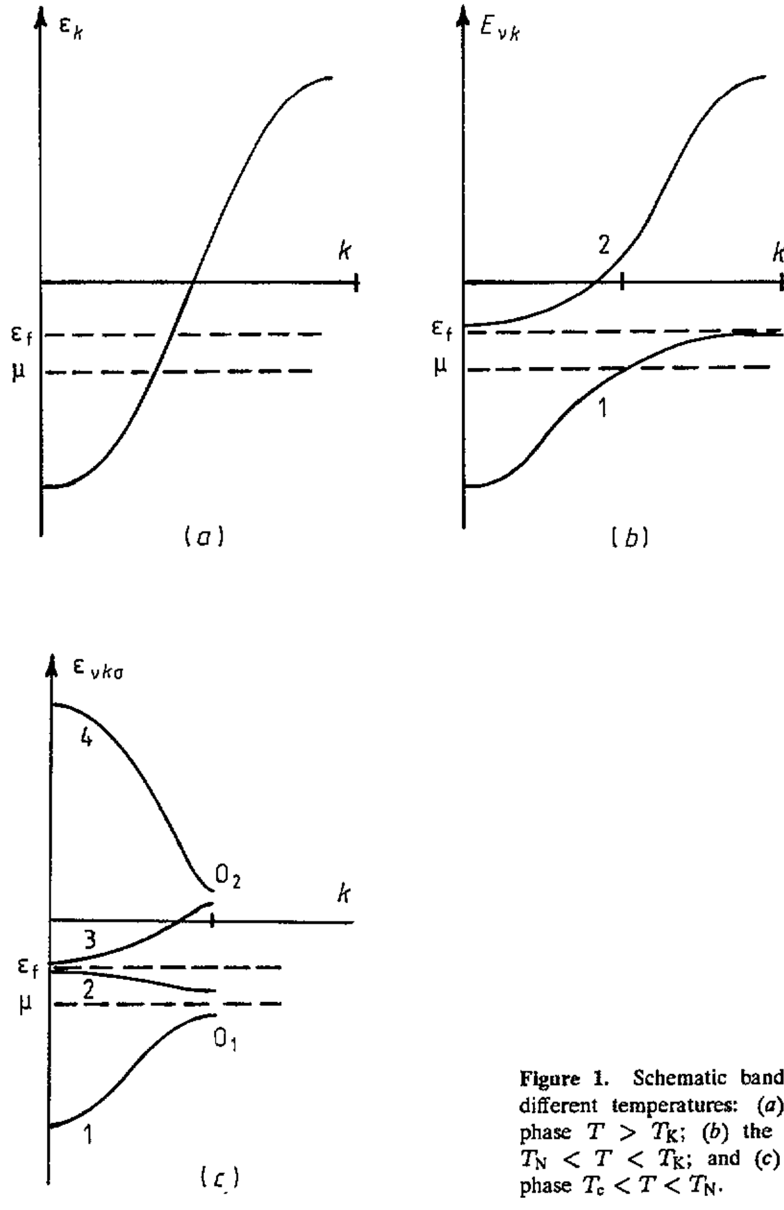

Figure 1. Schematic band structure diagram at different temperatures: (*a*) the high-temperature phase $T > T_{\rm K}$; (*b*) the coherent Kondo state $T_{\rm N} < T < T_{\rm K}$; and (*c*) the antiferromagnetic phase $T_{\rm c} < T < T_{\rm N}$.

At $T < T_{\rm K}$ the energy spectrum consists of the two N-fold degenerate bands (see figure 1(*b*))

$$E_{1k} = \tfrac{1}{2}\{\epsilon_k + \epsilon_{\rm f} - [(\epsilon_k - \epsilon_{\rm f})^2 + 4b^2]^{1/2}\}$$
$$E_{2k} = \tfrac{1}{2}\{\epsilon_k + \epsilon_{\rm f} + [(\epsilon_k - \epsilon_{\rm f})^2 + 4b^2]^{1/2}\}. \quad (5)$$

Since $n_{\rm f} = 1/2$, the low band E_{1k} is half full. The oper ators $f_{\sigma k}$ and $c_{\sigma k}$ are related to the annihilation operators $b_{1\sigma k}$ and $b_{2\sigma k}$ of the bands (5) by the Bogoliubov transformation

$$c_{\sigma k} = \sum_{\nu=1,2} u_{\nu k} b_{\nu\sigma k}$$
$$f_{\sigma k} = \sum_{\nu=1,2} v_{\nu k} b_{\nu\sigma k}$$
$$u_{1k} = v_{2k} = \cos\alpha_k \tag{6}$$
$$u_{2k} = -v_{1k} = \sin\alpha_k$$
$$\cot\alpha_k = (\epsilon_f - E_{1k})/b.$$

Let the non-renormalized band ϵ_k satisfy the nesting condition with respect to the middle of the band. In measuring the energy at the middle of the band, we can write

$$\epsilon_k = -\epsilon_{k-Q}. \tag{7}$$

Below we consider only the simplest case $Q = (\pm\pi, \pm\pi, \pm\pi)$. Using (7) and $n_t = 1/2$, one can show that the band E_{1k} possesses nesting regarding the Fermi level, that is

$$E_{1k} - \mu = -E_{1k-Q} + \mu \tag{8}$$

in such a range of k near k_F where electrons have the enhanced mass $m^* = m_0 \cos^{-2}\alpha_F$. The nesting (8) leads to the instability of the coherent Kondo state with respect to the antiferromagnetic ordering of the localized moments. At $T < T_K$ the antiferromagnetic state is characterized by the following thermodynamic average values

$$J_1\psi_i \equiv h_i = -J_1 N^{-1}\langle s_i^z\rangle = h\exp(iQR_i)$$
$$\psi_i^* \equiv M_i = N^{-1}\langle S_i^z\rangle = M\exp(iQR_i) \tag{9}$$

where h_i is the spontaneous magnetic field acting on the localized moment S_i^z [11]. The antiferromagnetic ordering brings about a reconstruction of the energy spectrum (5). The bands (5) are split at k lying on the Fermi surface. Instead of two N-fold degenerate bands (see figure 1(c)) we obtain four families of two fold degenerate bands (see figure 1(c))

$$\mathcal{E}_{1k\sigma} = \tfrac{1}{2}\left\{E_{1p} + E_{1k} - \left[(E_{1p} - E_{1k})^2 + 4t_\sigma^2\right]^{1/2}\right\}$$
$$\mathcal{E}_{2k\sigma} = \tfrac{1}{2}\left\{E_{1p} + E_{1k} + \left[(E_{1p} - E_{1k})^2 + 4t_\sigma^2\right]^{1/2}\right\}$$
$$\mathcal{E}_{3k\sigma} = \tfrac{1}{2}\left\{E_{2p} + E_{2k} - \left[(E_{2p} - E_{2k})^2 + 4z_\sigma^2\right]^{1/2}\right\} \tag{10}$$
$$\mathcal{E}_{4k\sigma} = \tfrac{1}{2}\left\{E_{2p} + E_{2k} + \left[(E_{2p} - E_{2k})^2 + 4z_\sigma^2\right]^{1/2}\right\}$$
$$t_\sigma = \frac{\sigma}{N}\left(h - J_1 M m_0/m^*\right)$$
$$z_\sigma = \frac{\sigma}{N}\left(h m_0/m^* - J_1 M\right)$$

where $p = k - Q$. At low temperatures, $T \ll T_K$, we have $m^*/m = \cos^{-2}\alpha_F = q_0/\rho_0 t_0 \gg 1$ [13, 14]. The energy T_0 is determined by the equality $T_0 = \epsilon_f - \mu$, and at $T \ll T_K$ it acts as a universal energy scale [13, 14]:

$$T_0 = n_c \rho_0^{-1} \exp\left(\frac{-1}{J\rho_0}\right). \tag{11}$$

Equations (10) and (11) are correct at k near the boundaries of the reduced Brillouin band (the points O_1 and O_2 in figure 1(*c*)). The Néel temperature T_N has been obtained in [11]

$$T_N = T_0 \exp\left(\frac{-T_0}{A\alpha^2 J_1^2 \rho_0 q_0}\right) \tag{12}$$

where $\alpha = j(j+1)/3N^2$; A is a certain number parameter which depends weakly on the parameters of the model. Solving self-consistently the set of saddle-point equations, at $T \ll T_N$ we obtain

$$\begin{aligned} h &= T_N \\ M &= \alpha q_0 \left(\frac{T_N}{T_0}\right) \ln\left(\frac{T_0}{T_N}\right). \end{aligned} \tag{13}$$

According to (9) and (13), the antiferromagnetic moment per f-atom is equal to

$$\begin{aligned} M_a &= g_j \mu_B N M \\ &= g_j \mu_B Q_0 \frac{j(j+1)T_N}{3N^2 T_0} \ln \frac{T_0}{T_N} \end{aligned} \tag{14}$$

where $Q_0 = q_0 N$ is the total number of f-electrons per f-atom. For UPt_3 experiment yields T_N = 5.5 K [8], j = 5/2 and g_j = 6/7 [3], Q_0 = 1. The value of T_0 is not exactly known and probably lies in the range 20 K $< T_0 <$ 50 K [3]. For these experimental data equation (14) gives 0.028 $\mu_B > M_a >$ 0.02 μ_B. Our estimate is in surprisingly good agreement with the experimental result 0.02 μ_B per U-atom of [8]. For URu_2Si_2 T_N = 17 K (see for example [4]). If we use $T_0 \sim$ 50 K (the temperature at which the susceptibility and resistivity pass through a maximum [4]) and j = 1/2, g_j = 2, then we obtain M_a = 0.046 μ_B. This result is close to the experimental value 0.04 μ_B [9, 10].

In the case $n_t = n_c + q_0 < 1/2$ at $T \ll T_N$, the low antiferromagnetic bands $\mathcal{E}_{1k\sigma}$ are not completely filled. The value $\delta = 1/2 - n_t$ is the number of holes per orbital. At $\delta \neq 0$ the nesting condition (8) cannot be exact, but at $\delta \ll q_0 T_N/T_0$ the approximate nesting is sufficient for the development of the antiferromagnetic state with $Q = (\pm\pi, \pm\pi, \pm\pi)$ and the energy bands of (10).

Now we consider the stability of our model with respect to fluctuations Δ_i^* and Δ_i (see equation (4)). One can find that in the range $T_N < T < T_K$ the Kondo screening suppresses completely the fluctuations Δ. However, at $T < T_N$ the antiferromagnetic ordering revives these fluctuations leading to instability of the antiferromagnetic state with respect to superconductivity. Considering only the static fluctuation of Δ_i^* and Δ_i, we select from (4) the operator

$$\begin{aligned} \rho &= \sum_{\sigma i}\left(\Delta_i f_{\sigma i}^{+} c_{-\sigma i}^{+} + \mathrm{HC}\right) \\ &= \sum_{q,k}\left(\Delta_q f_{\sigma k}^{+} c_{-\sigma, q-k}^{+} + \mathrm{HC}\right) = \sum_q \rho_q . \end{aligned} \tag{15}$$

Due to the symmetry of the system considered we can expect an instability either in the channel $q = 0$ or in the antiferromagnetic channel $q = Q$. To find the instability, we transform the f– and c-operators into operators $a_{\nu\sigma k}$ of the bands (10). For this purpose we must find a unitary transformation which diagonalizes the effective Hamiltonian describing the antiferromagnetic state. The Hamiltonian may be written as

$$H = \sum \begin{pmatrix} b^+_{1\sigma k} \\ b^+_{1\sigma p} \\ b^+_{2\sigma k} \\ b^+_{2\sigma p} \end{pmatrix} \begin{pmatrix} E_{1k} & A^{11}_\sigma & 0 & A^{12}_\sigma \\ A^{11}_\sigma & E_{1p} & A^{21}_\sigma & 0 \\ 0 & A^{21}_\sigma & E_{2k} & A^{22}_\sigma \\ A^{12}_\sigma & 0 & A^{22}_\sigma & E_{2p} \end{pmatrix} \begin{pmatrix} b_{1\sigma k} \\ b_{1\sigma p} \\ b_{2\sigma k} \\ b_{2\sigma p} \end{pmatrix} \tag{16}$$

$$A^{\nu\mu}_\sigma = -\frac{\sigma}{N} h v_{\nu k} v_{\mu p} + \frac{\sigma}{N} J_1 M u_{\nu k} u_{\mu p} \tag{17}$$

where the functions v, u and operators b are given by (6). Using the perturbation theory with respect to the matrix elements A^{12} and A^{21} up to first order, we obtain the spectrum (10), the unitary transformation and then the following relations between operators $b_{\nu k}$ and operators $a_{1\sigma k}$ of the low antiferromagnetic bands:

$$\begin{aligned} b_{1\sigma k} &= a_{1\sigma k} \cos\beta_{\sigma k} + \dots \\ b_{1\sigma p} &= a_{1\sigma k} \sin\beta_{\sigma k} + \dots \\ b_{2\sigma k} &= -a_{1\sigma k} A^{21}_\sigma E_g^{-1} \sin\beta_{\sigma k} + \dots \\ b_{2\sigma p} &= -a_{1\sigma k} A^{12}_\sigma E_g^{-1} \cos\beta_{\sigma k} + \dots \end{aligned} \tag{18}$$

where

$$\begin{aligned} E_g &\approx E_{2k_F} - E_{1k_F} \approx \frac{q_0}{\rho_0} \\ ms\cos\beta_{\sigma k} &= \frac{E_{1p} - \mathcal{E}_{1k\sigma}}{D} \\ \sin\beta_{\sigma k} &= -\frac{A^{11}_\sigma}{D} \\ D &= \left[(E_{1p} - \mathcal{E}_{1k\sigma})^2 + \left(A^{11}_\sigma\right)^2 \right]^{1/2}. \end{aligned} \tag{19}$$

Substituting (6) and (18) into (15), one obtains

$$P_Q = \sum_{\sigma k} \left(\Delta_{\sigma k} a^+_{1\sigma k} a^+_{1,-\sigma,-k} + \text{HC} \right) + \rho_F \tag{20}$$

$$\Delta_{\sigma k} = -\frac{\sigma}{N} \Delta_Q \frac{J_1 M}{E_g} \left(\frac{m_0}{m^*} \right)^{1/2} \cos 2\beta_{\sigma k} \tag{21}$$

where the operator ρ_F contains all other combinations of the operators $a_{\nu\sigma k}$. To derive (22) we have used $m^*/m_0 \gg 1$ and the inequality $J_1 M \gg h$. The instability of the antiferromagnetic state with respect to the superconducting transition is completely determined by the first term of the operator (20). The operator ρ_F gives a non-singular contribution. Equation (21) shows that the superconducting vertex is proportional to the antiferromagnetic moment M. Thus at $T > T_N$ we have $M = 0$ and there is no superconductivity. The temperature T_c of the superconducting transition is given by the equation

$$\frac{1}{J_2} = \frac{1}{N}\sum_{\sigma}\int \frac{\mathrm{d}k}{(2\pi)^d}\left(\frac{\partial\Delta_{\sigma k}}{\partial\Delta_Q}\right)^2 \frac{th[(\mathcal{E}_{1k\sigma} - \mu)/2T]}{\mathcal{E}_{1k\sigma} - \mu} \tag{22}$$

where the vertex renormalization $\partial\Delta_{\sigma k}/\partial\Delta_Q$ follows from (21). In the case $T_c \ll T_N \ll T_0$ and $N \gg 1$ we find

$$T_c = \mu_c \exp\left(-\frac{4E_g^2 h^3}{\pi J_1^2 M^2 J_2 \rho_0 \mu_c^3}\right) \tag{23}$$

where

$$\mu_c = [2\delta T_0 T_N/\pi q_0]^{1/2}$$

acts as the effective chemical potential for holes in the bands $\mathcal{E}_{1k\sigma}$. According to (23), T_c increases rapidly with increasing hole concentration δ. On the other hand, increasing δ results in the violation of the nesting (8) and decreases T_N. At large δ this process will lead to decreasing T_c. It is necessary to note that at finite N the δ-dependence of T_c can differ from (23).

We can assume that if the antiferromagnetic gap $t_{\sigma k}$ is equal to zero in some directions of k, then the superconducting gap $\Delta_{\sigma k}$ is equal to zero also. This assumption allows us to explain the power law temperature-dependence of the specific heat of the heavy-fermion compounds at $T < T_c$ [1–4].

In conclusion, we have shown that in the framework of the mean-field theory (large N-limit) the model (1) has a rich phase diagram which includes a coherent Kondo state, magnetically ordered phases and superconductivity. The superconductivity is driven by the exchange interaction between conduction electrons and localized f-electrons and can occur only at $T_c < T_N < T_K$, that is in the coherent Kondo state with antiferromagnetically ordered localized moments.

References

[1] Brandt N B and Moshchalfov V V 1984 *Adv. Phys.* **33** 373

[2] Stewart G R 1985 *Rev. Mod. Phys.* **56** 755

[3] De Visser A, Menovsky A and France J J M 1987 *Physica* B & C **147** 81

[4] Rauchschwalbe U 1987 *Physica* B & C **147** 1

[5] *Proc. 6th Int. Conf. on Valence Fluctuations* 1991 *Physica* B **171**

[6] Chen J W, Lambert S E, Maple M B, Fisk Z, Smith J L, Stewart G R and Willis J O 1984 *Phys. Rev.* B **30** 1583

[7] Maple M B, Chen J W, Lambert S E, Fisk Z, Smith J L, Ott H R, Brooks J S and Naughton M J 1985 *Phys. Rev. Lett.* **54** 477

[8] Aeppli G, Bucher E, Broholm C, Kjems J K, Baumann J and Haufnagl J 1988 *Phys. Rev. Lett.* **60** 615

[9] Broholm C, Kjems J K, Buyers W J L, Matthews P, Palstra T T M, Menovsky A A and Mydosh J A 1987 *Phys. Rev. Lett.* **58** 1467

[10] Mason T E, Gaulin B D, Garrett J D, Tun Z, Buyers W J L and Isaacs E D 1990 *Phys. Rev. Lett.* **65** 3189
[11] Goltsev A V 1992 *J. Phys.: Condens. Matter* submitted
[12] Coqblin B and Schrieffer J R 1969 *Phys. Rev.* **185** 847
[13] Newns D W and Read N 1987 *Adv. Phys.* **34** 799
[14] Belitsky V I and Goltsev A V 1991 *Physica* B **172** 459