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LETTER TO THE EDITOR

Superconductivity due to ferromagnetically ordered localized spins

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Abstract

A new mechanism of simultaneous appearance of ferromagnetism and superconductivity based on interaction of electrons mediated by localized spins was recently proposed by Suhl. Here the superconducting critical temperature is calculated for this model and conditions for appearance of superconductivity are analysed. It is shown that this mechanism can lead only to an s-wave order parameter. Superconductivity appears together with ferromagnetism but persists only until the ferromagnetism is weak. In order for it not to be destroyed by the paramagnetic effect, the metal has to be of a heavy-fermion type. This all fits recent experimental data obtained for UGe₂.

1. Introduction

Recently a very strange phenomenon has been observed: superconductivity appearing simultaneously with ferromagnetism (see [1, 2], and references therein). According to conventional ideas, these two phenomena are incompatible, since, due to the paramagnetic (Clogston) effect, the magnetization tends to flip the spins of the Cooper pair to make them parallel to the magnetic induction. If the pairing is associated with exchange of quasiparticles with a large momentum, like phonons in conventional superconductors, the interaction is virtually local, and leads to an s pairing with a singlet order parameter. In order to have triplet pairing, which could be compatible with ferromagnetism, the interaction has to be sufficiently non-local. There is, however, also another concern. Until recently all the models of superconductivity assumed that the quasiparticles mediating the Cooper pairing belong to a system different from conduction electrons, e.g., phonons, magnons in a system of localized spins, etc. The attempts to construct superconductivity within the same electron system as is responsible for the ferromagnetism (see [3–5] and references therein) are not very convincing and lead sometimes to predictions contradicting the experiment.

In this connection it is necessary to consider the experimental results more thoroughly. The F–SC combination was first observed in UGe₂ under pressure [1, 6, 7]. There are some characteristic features of this material and of the experimental results. First of all, the magnetic

moment of uranium is due to f shells, and, therefore, it can be considered as localized. The experiments on high-purity single crystals and on polycrystals give essentially the same results, and this is irrefutable evidence that the pairing is in the s state—the only one not destroyed by scattering from potential impurities. In contrast to that, the material $ZrZn_2$, where also the F–SC combination was recently observed [2], has much less localized d electrons. Superconductivity is observed only in extremely pure samples, and a rather weak disorder destroys it completely. Therefore, it is very likely that there is a p-wave pairing, and it is described by one of the models of [3–5]. The overall conclusion is that one should not try to squeeze everything into one particular mechanism, as has happened in the past with the so-called 'unconventional' superconductors, such as organics, bucky-balls, high- T_c superconductors, etc.

I will further concentrate on UGe₂. A very interesting concept of superconductivity in this substance was proposed recently by Suhl [8], who suggested that an s-wave superconductivity could result from the interaction of electrons mediated by ferromagnetically ordered localized spins. In [8] a Cooper-type derivation was performed with somewhat obscure calculations, which gave only a hint at the possibility of superconductivity, just like Cooper's original paper [9]. Therefore, I felt it worthwhile to perform a rather standard type of calculation of the critical temperature within the model [8], taking into account not a single localized spin but the whole ensemble, and, also, not a single pair but the whole electron system. This calculation confirmed Suhl's idea, and it will be presented in the following sections together with some analysis.

2. Critical temperature

I will use the simplest model of an interaction of electrons with localized spins:

$$I\sum_{n}\sigma(r_{n})S_{n}.$$
(1)

The electron spin density will be described by the usual operators:

$$\sigma^{i}(\mathbf{r}) = \sum_{\alpha,\beta} \psi^{+}_{\alpha}(\mathbf{r}) \sigma^{i}_{\alpha\beta} \psi_{\beta}(\mathbf{r})$$
⁽²⁾

 $(\sigma^i_{\alpha\beta}$ are the Pauli matrices), and the localized spins by the 'pseudo-fermions' [10, 11]:

$$S_n^i = \sum_{M,M'=-S}^{S} a_{nM}^+ S_{MM'} a_{nM'}.$$
(3)

Since the papers [10, 11] are not easily accessible, I will mention here that if the operators a_{nM} have the usual fermion commutation relations, and $S_{MM'}^i$ are the spin matrices, the operators, S_n^i , will have the necessary commutation relations for spin operators. Such a presentation introduces, however, in addition to 'physical' states, where only one state is occupied (one of the numbers $n_M = 1$, and the others are 0), some 'unphysical' states, where several of the occupation numbers are non-zero, or all are zero. They can be excluded by the following procedure. First of all, any operator S_n^i , or a product of several such operators, gives zero, acting on the state with no 'particles' in any of the *M*-states. The states with two, or more, 'particles' can be excluded by introduction of a large 'energy' λ per 'particle', i.e., adding to the Hamiltonian the term

$$\lambda \sum_{M=-S}^{S} n_M.$$

If $\lambda \to 0$, the 'many-particle terms' will be smaller than the 'physical' terms. In order to get the correct average, one has to multiply the result by the factor $e^{\lambda/T}/(2S+1)$, or, in the presence of

$$\Gamma = \underbrace{\underbrace{}}_{1} + \underbrace{\underbrace{}}_{1} +$$

Figure 1. Ladder diagrams to be summed for the definition of T_c . The thick lines correspond to electron Green functions, the thin lines to Green functions of pseudo-fermions; the vertices correspond to the interaction of electrons with localized spins (formula (1)).

a magnetic field, by $e^{\lambda/T} \sinh(H/2T) / \sinh[H(S + 1/2)/T]$, per participating localized spin (here *H* is the equivalent of μH).

According to what was said before, the Hamiltonian is

$$H = J \sum_{n} \sum_{M,M'=-S}^{S} \sum_{\alpha,\beta} a_{n,M}^{+} S_{MM'} a_{n,M'} \psi_{\alpha}^{+}(\mathbf{R}_{n}) \sigma_{\alpha\beta} \psi_{\beta}(\mathbf{R}_{n}) - H \sum_{n} \sum_{M=-S}^{S} \sum_{\alpha,\beta} a_{n,M}^{+} M a_{n,M}$$
$$- h \int dV \sum_{\alpha,\beta} \psi_{\alpha}^{+}(\mathbf{r}) \sigma_{\alpha\beta}^{z} \psi_{\beta}(\mathbf{r}) + \lambda \sum_{n} \sum_{M=-S}^{S} a_{n,M}^{+} a_{n,M}$$
(4)

where it was supposed that 'exchange fields' h and H are acting on electrons and localized spins (their origin will be discussed in the next section). Following the general rule (see [10], section 33, subsection 3), it is necessary to find the pole of the sum of the ladder diagrams shown in figure 1 with zero total incoming frequency and momentum, where the thin lines stand for pseudo-fermions. Every 'step' of the ladder is equal either to

$$J^{2} \sum_{n} \sum_{M=-S}^{S} M^{2}T \sum_{\omega} (i\omega + MH - \lambda)^{-1} [i(\omega + \Omega) + MH - \lambda]^{-1}$$
(5)

with no change of the electron spin, or to

+
$$J^{2} \sum_{n} \sum_{M=-S}^{S} (S - M + 1)(S + M)T \sum_{\omega} (i\omega + MH - \lambda)^{-1} [i(\omega + \Omega) + (M - 1)H - \lambda]^{-1}$$

(6)

with the electron spin changing from 1/2 to -1/2 in the upper line and inversely in the lower line, or vice versa. Here $\omega = \pi (2n + 1)$, $\Omega = 2\pi m$. It is easy to see that the sum over ω in (5) is finite only for $\Omega = 0$, and that it does not lead to a logarithmically large quantity, since there is no summation over electron frequencies. In (6) we get a finite result for a finite Ω .

Performing the summation over ω and M for a given n, multiplying by $e^{\lambda/T} \sinh(H/2T)/\sinh[H(S+1/2)/T]$, and putting $\lambda \to \infty$, we obtain

$$2J^2 SB_S(H/T)(i\Omega + H)^{-1}.$$
(7)

Here $B_S(H/T)$ is the Brillouin function

$$B_{S}(H/T) = \frac{S+1/2}{S} \operatorname{coth}[(S+1/2)H/T] - \frac{1}{2S} \operatorname{coth}[H/(2T)].$$
(8)

The localized spins in every step must be different, since otherwise every loop will give a factor $\exp(-\lambda/T)$ and there will be only one compensating factor $\exp(\lambda/T)$. Since at $T \to T_c$ the coherence length becomes infinite, the absence of some spins from the whole sum makes no difference. The summation over the localized spins can be therefore replaced by a volume integration: $\sum_n \to N \int dV$, where *N* is the density of localized spins.

In order to get a non-vanishing result, the electrons between the steps must be supposed to have different polarizations, and, hence, the superconducting ordering under consideration has to be *singlet*. The product of the electron Green functions is

$$(\omega - \Omega) + h - \xi]^{-1} [-\mathbf{i}(\omega - \Omega) - h - \xi]^{-1}$$

The main logarithm appears if $h \ll H$, and is the result of an integration over ξ and summation over $\omega' = \omega - \Omega$ in the region $h \lesssim \omega' \ll H$. Therefore in the factor $(i\Omega + H)^{-1}$ we can neglect Ω , and what remains is

$$\frac{\omega T}{H} \sum_{|\omega'| \ll H} \int \mathrm{d}\xi \left[\xi^2 + (\omega' - \mathrm{i}h)^2\right]^{-1}$$

where v is the density of states:

[i

$$\nu = \frac{p_0 m}{2\pi^2}.\tag{9}$$

Integration with respect to ξ results in

$$\frac{\partial \pi}{H} \sum_{0 < \omega' < H} \left[(\omega' - \mathrm{i}h)^{-1} + (\omega' + \mathrm{i}h)^{-1} \right].$$

After some simple transformations we obtain

$$\frac{\nu}{H} \left[\ln \frac{2\gamma H}{\pi T} + \psi \left(\frac{1}{2} \right) - \frac{1}{2} \psi \left(\frac{1}{2} - \frac{\mathrm{i}h}{2\pi T} \right) - \frac{1}{2} \psi \left(\frac{1}{2} + \frac{\mathrm{i}h}{2\pi T} \right) \right]$$

where ψ is the digamma function.

Summation of the whole ladder gives

$$\Gamma = 2J^2 N S[B_S(H/T)/H] \left\{ 1 - 2J^2 N \nu S[B_S(H/T)/H] \times \left[\ln \frac{2\gamma H}{\pi T} + \psi \left(\frac{1}{2} \right) - \frac{1}{2} \psi \left(\frac{1}{2} - \frac{ih}{2\pi T} \right) - \frac{1}{2} \psi \left(\frac{1}{2} + \frac{ih}{2\pi T} \right) \right] \right\}.$$
 (10)

This expression has a pole, which defines the critical temperature as a function of H and h. In order to understand more clearly the limiting cases, we use the integral form of the digamma function:

$$\psi(z) = \int_0^\infty \left(\frac{e^{-t}}{t} - \frac{e^{-zt}}{1 - e^{-t}}\right) \, \mathrm{d}t. \tag{11}$$

The equation for T_c transforms to

$$2J^2 N \nu S[B_S(H/T_c)/H] \left(\ln \frac{2\gamma H}{\pi T_c} - \int_0^\infty \frac{1 - \cos(hz/\pi T_c)}{\sinh z} \, \mathrm{d}z \right) = 1 \quad (12)$$

where $\gamma = e^C \simeq 1.78$. For the case h = 0 we get

$$2J^2 N \nu S[B_S(H/T_c)/H] \ln \frac{2\gamma H}{\pi T_c} = 1.$$
⁽¹³⁾

Since, strictly speaking, our derivation is valid only for $T_c \ll H$, we can substitute $B_S(H/T_c) \simeq 1$ and get

$$T_c \simeq \frac{2\gamma H}{\pi} \exp\left(-\frac{H}{2J^2 N \nu S}\right). \tag{14}$$

If we try to extrapolate to $T_c \sim H$, the square bracket in (13) will not depend on H, and we can conclude that in this region T_c grows linearly with H. After a maximum at $H = J^2 N \nu S/2$, it decreases with H. This shows that without the exchange field there is no new mechanism for

superconductivity. At the same time H must not be too large; otherwise, superconductivity will be suppressed. This fits the experimental data qualitatively [1].

In contrast to the exchange field acting on the localized spins, the field acting on the electrons has a negative effect. Returning to formula (12), we obtain for $h \ll T_c$

$$T_c \simeq T_{c0} - \frac{7\zeta(3)}{4\pi^2} \frac{h^2}{T_{c0}}$$
(15)

where T_{c0} is the value given by formula (14). In the opposite limiting case, $h \gg T_{c0}$, the integral in (12) is equal to $\ln(2\gamma h/\pi T_c)$ and we get the formula

$$\frac{1}{2}J^2 N \nu S[B_S(H/T_c)/H] \ln(H/h) = 1.$$
(16)

It is easy to see that if h exceeds T_{c0} , this equation has no solutions.

3. Exchange fields

Until now we have treated the exchange fields, H and h, as some given quantities, and did not consider their origin. The conclusion that we have reached is that superconductivity mediated by local moments can exist only if $H > T_c > h$. The question that arises is: is this possible? The exchange field H can appear as a result of the interaction of the localized spins with the spins of electrons (1) but it can also have another origin, such as direct exchange or superexchange. Independently of this, the maximum possible critical temperature $T_{c,max} \sim J^2 N \nu S$. On the other hand, it is hard to imagine any source of h not associated with localized spins. Therefore

$$h = JNSB_S(H/T)$$

and, at $H > T_c$, $h \sim JNS$. Since this has to be less than T_c , we get the following condition: $J\nu \gg 1.$ (17)

This condition was also obtained in [8]. Since the exchange energy is always somewhat less than the main electronic energies, the only possibility is a large density of states, ν . According to formula (9), this can happen only for a large effective mass, i.e., if the substance is a heavy-fermion metal. This agrees with the estimate in [1] based on the results for the resistivity and specific heat, namely, $m \sim 50m_e$.

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