Nonmagnetic impurities in magnetic superconductors

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The magnetic moment which arises around a nonmagnetic impurity in a magnetic superconductor with triplet pairing is derived. An interpretation is offered for some μSR experiments which have been carried out to measure the local magnetic moments in the superconducting phases of the heavy-fermion compound $U_{1-x}Th_xBe_{13}$.

Among the superconducting phases which belong to nontrivial superconducting classes, there are some with a broken symmetry with respect to time reversal.[1] In such phases, the magnetic moment of a Cooper pair,

$$\vec{\mu}_k = \mathrm{Sp}\Delta^+\vec{\sigma}\Delta + \mathrm{Sp}\hat{\Delta}^+\frac{1}{i}[\mathbf{k}\times\frac{\partial}{\partial\mathbf{k}}]\,\Delta\,, \qquad (1)$$

is nonzero. Here Δ is the order parameter of the superconductor, given by $\Delta = \boldsymbol{\sigma}\mathbf{d}(\mathbf{k})i\sigma_y$ for triplet pairing and by $\Delta = \psi(\mathbf{k})i\sigma_y$ for singlet pairing; the functions

$\mathbf{d}(\mathbf{k})$ and $\psi(\mathbf{k})$ are linear combinations of the basis functions of irreducible representations of the symmetry group of the crystal; and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices. Some of the superconducting phases having a $\boldsymbol{\mu}_k$ are ferromagnetic $\int \boldsymbol{\mu}_k dS_k \neq 0$, while others are antiferromagnetic $\int \boldsymbol{\mu}_k dS_k = 0$; $\int dS_k$ means an integration over the entire Fermi surface). As we know from the theory of superfluid ^{3}He, the density of either a spin magnetic moment[2] or an orbital magnetic moment[3] of a ferromagnetic phase is an extremely small quantity:

$$\mathbf{m} \propto \mu_B n(\Delta(T)/\epsilon_F)^2 \hat{\boldsymbol{\mu}} \tag{2}$$

Here μ_B is the Bohr magneton, n is the density of conduction electrons, ε_F is the Fermi energy, $\Delta(T)$ is the gap in the excitation spectrum, and the unit vector $\boldsymbol{\mu}$ is directed along $\int \boldsymbol{\mu}_k dS_k$. This moment, like the magnetic moment which arises in a magnetic superconductor as a result of surface currents and which has a significantly larger value, $\sim\mu_B/2$ per conduction electron,[4] is completely canceled in the interior of a homogeneous superconductor by the Meissner current.[1]

Any irregularity of atomic scale (an impurity or a defect) leads to changes in the electron wave functions and also in the order parameter near the impurity.[5] As a result, an additional magnetic moment appears. This magnetic moment is concentrated around the impurity in a volume with a size on the order of the coherence length ξ_0:

$$\mathbf{M}_i \propto \mathbf{m}\frac{\sigma_{tot}}{\xi_0^2}\xi_0^3 \propto \mu_B \frac{\Delta^2}{\epsilon_F T_c}\sigma_{tot} k_F^2 \hat{\boldsymbol{\mu}}. \tag{3}$$

Here σ_{tot} is the total cross section for electron scattering by an impurity in the normal metal, and T_c is the transition temperature. The magnetic field which corresponds to this moment is screened over distances on the order of the London penetration depth, which is considerably greater than ξ_0.

Both undamped ring currents and the perturbation of the spin density around an impurity contribute to magnetic moment (3). An important point is that the spatial distribution of the spin density around an impurity in a superconductor with triplet pairing oscillates in the manner of the spin density around a magnetic impurity in a normal metal (RKKY). The density of the magnetic moment at the position of the impurity and thus the strength of the magnetic field H_{sp} at this point are therefore given in order of magnitude by

$$\mathbf{m}_i(\mathbf{r}=0) \propto \mathbf{H}_{sp}(\mathbf{r}=0) \propto n\mathbf{M}_i\,. \tag{4}$$

The magnetic field induced by undamped ring currents, which was found in Ref. 6, is weaker by a factor of T_c/ε_F:

$$\mathbf{H}_{orb}(\mathbf{r}=0) \propto \frac{T_c}{\epsilon_F}\mathbf{H}_{sp}(\mathbf{r}=0). \tag{5}$$

The validity of (3) and (4) can be verified by calculating the density of the spin magnetic moment induced by the impurity, from the formula

$$\mathbf{m}_i(\mathbf{r}) = \frac{\mu_B}{4} T \sum_\omega \iint \frac{d^3k_1}{(2\pi)^3} \frac{d^3k_2}{(2\pi)^3} e^{i(\mathbf{k}_1 - \mathbf{k}_2)\mathbf{r}} \; \mathrm{Tr}_\sigma \vec{\sigma} \mathrm{Sp}_\tau \tau_3 (\hat{G}_\omega(\mathbf{k}_1\mathbf{k}_2) - \hat{G}^S_\omega(\mathbf{k}_1)\delta(\mathbf{k}_1 - \mathbf{k}_2)). \tag{6}$$

Here

$$\hat{G}_\omega(\mathbf{k}_1\mathbf{k}_2) = \hat{G}^S_\omega(\mathbf{k}_1)\delta(\mathbf{k}_1 - \mathbf{k}_2) + \hat{G}^S_\omega(\mathbf{k}_1)\hat{T}_{\mathbf{k}_1\mathbf{k}_2}\hat{G}^S_\omega(\mathbf{k}_2) \tag{7}$$

is the matrix Green's function of a superconductor with an impurity.[1)] Each of the four Green's functions in the matrix $\hat{G}_\omega(\mathbf{k}_1\mathbf{k}_2)$ is itself a (2×2) matrix in spin space. The operations Tr_τ and Tr_σ take the trace over the indices of the matrices in respectively particle-hole space and spin space;

$$\hat{G}^S_\omega(\mathbf{k}) = \frac{(-i\omega\tau_0 - \xi\tau_3 + \hat{\Delta})((\xi^2 + \omega^2 + \mathbf{dd}^*)\tau_0 - i[\mathbf{d}\times\mathbf{d}^*]\hat{\mathbf{A}})}{(\xi^2 + \omega^2 + \mathbf{dd}^*)^2 + [\mathbf{d}\times\mathbf{d}^*]^2} \tag{8}$$

is the matrix Green's function of a superconductor without an impurity. Here $\boldsymbol{\tau} = (\tau_1,\tau_2,\tau_3)$ are the Pauli matrices in particle-hole space, $\hat{\mathbf{A}} = \begin{pmatrix}\sigma & 0\\ \sigma & -\sigma_y\sigma\sigma_y\end{pmatrix}$, τ_0 is the unit matrix, $\hat{\Delta} = \begin{pmatrix}0 & \Delta\\ \Delta^+ & 0\end{pmatrix}$ is the order-parameter matrix, and $\Delta = i\sigma d(k)\sigma_y$. The exact matrix scattering amplitude for scattering by the impurity,

$$\hat{T}_{k_1k_2} = \begin{pmatrix} T_{k_1k_2} & 0 \\ 0 & -T^*_{-\mathbf{k}_2\,-\mathbf{k}_1}\end{pmatrix}$$

is related to the exact matrix scattering amplitude for a scattering by an impurity in a normal metal,

$$\hat{T}^N_{\mathbf{k}_1\mathbf{k}_2} = \begin{pmatrix} T^N_{\mathbf{k}_1\mathbf{k}_2} & 0 \\ 0 & -T^{N*}_{-\mathbf{k}_2-\mathbf{k}_1}\end{pmatrix}; \quad T^N_{\mathbf{k}_1\mathbf{k}_2} = -\frac{1}{\pi N_0}\sum_{l=0}^{\infty} \sin\delta_l e^{i\delta_l} l P_l(\hat{\mathbf{k}}_1\hat{\mathbf{k}}_2),$$

by the equation

$$\hat{T}_{\mathbf{k}_1\mathbf{k}_2} = \hat{T}^N_{\mathbf{k}_1\mathbf{k}_2} + \int \frac{d^3k_3}{(2\pi)^3} \hat{T}^N_{\mathbf{k}_1\mathbf{k}_3}(\hat{G}^S_\omega(\mathbf{k}_3) - \hat{G}^N_\omega(\mathbf{k}_3))\hat{T}_{\mathbf{k}_3\mathbf{k}_2}, \tag{9}$$

where $\hat{G}^N_\omega(k)$ is the matrix Green's function of the normal metal without an impurity.

For simplicity we consider a superconducting phase with p pairing, in which we have

$$d_\alpha(\hat{\mathbf{k}}) = \Delta(T)\sum_{\mu\nu} C_{\mu\nu}\lambda^\mu_\alpha\lambda^\nu_i\hat{k}_i, \qquad \lambda^{\pm1}_{\alpha,i} = \frac{\hat{x}_{\alpha,i} \pm \hat{y}_{\alpha,i}}{\sqrt{2}}, \quad \lambda^0_{\alpha,i} = \hat{z}_{\alpha,i}. \tag{10}$$

In the ferromagnetic A_1 phase, for example, only the coefficient $C_{11} = 1$ is nonzero. It is a straightforward matter to carry out calculations near T_c by expanding the Green's function $\hat{G}^S_\omega(\mathbf{k})$ in powers of $\Delta(T)$. As a result, we find the following expression for the total moment induced by the impurity:

$$\mathbf{M}_i = \int d^3 r \mathbf{m}_i(\mathbf{r}) = \frac{\mu_B}{16\pi} \frac{N_0'}{N_0} \frac{\Delta^2(T)}{T_c} k_F^2 (\sigma_{tot} - \sigma_{tr}) \cdot \frac{1}{3} \sum_{\mu\nu} \mu \,|C_{\mu\nu}|^2 \hat{\mathbf{z}}, \qquad (11)$$

This is a refinement of (3). Here N_0 and N_0' are the density of states and its derivative at the Fermi surface, and σ_{tot} and σ_{tr} are the total and transport cross sections for electron scattering by an impurity in the normal metal.

At the position of the impurity, moment density (6) contains many contributions of the same order of magnitude. Here is the expression for one of them, which corresponds to a term whose integral over the entire volume gives us total moment (11):

$$\mathbf{m}_i(\mathbf{r} = 0) = \frac{\mu_B}{16\pi} N_0' \epsilon_F \frac{\Delta^2}{T_c} k_F^2 (\sigma_{tot}^0 - \sigma_{tr}^0) \cdot \frac{1}{3} \sum_{\mu\nu} \mu |C_{\mu\nu}|^2 \hat{\mathbf{z}} \,. \qquad (12)$$

Here $\sigma_{tot}^0 - \sigma_{tr}^0 = (4\pi k_F^2)(t_0 t_1^* + t_1^* t_0)$, t_0 and t_1 are the partial s-wave and p-wave scattering amplitudes, and $t_l = \sin \delta_l e^{i\delta l}$. Expression (12) is literally the same as estimate (4).

Each impurity atom in a ferromagnetic superconductor with triplet pairing thus generates in its neighborhood a magnetic field which is oriented along the magnetic moment of the particular domain of the anisotropic superconductor[1] in which this atom lies. This field can be found by the method of muon spin rotation (μSR), by measuring the relaxation rate in a zero external field. Measurements of this type have been carried out on the heavy-fermion superconducting compound $U_{1-x}Th_xBe_{13}$ (Ref. 7), in which the superconducting transition splits in two at thorium concentrations $x > x_m \approx 1.7\%$ (Ref. 8). One possible explanation of this splitting starts from the assumption that the superconducting state of $U_{1-x}Th_xBe_{13}$ is a mixture of two superconducting phases, a and b, which belong to different representations[9] of the UBe_{13} symmetry group and which have different transition temperatures $T_{ca}(x)$ and $T_{cb}(x)$. These temperatures are of such a nature that the relation $T_{cb} > T_{ca}$ holds at $x < x_m$, while $T_{ca} > T_{cb}$ holds at $x > x_m$. The subordination scheme in Landau's theory of phase transitions describes only four different versions of pairs of phases a and b, for any of which the lower transition, on the line T_{cb}, is a first-order phase transition at $x > x_m$ (Ref. 10). One of these versions corresponds to a first-order transition between an antiferromagnetic phase belonging to superconducting class $O(D_2)$ and a ferromagnetic phase with symmetry $D_3(E)$. The abrupt appearance of the order parameter of a ferromagnetic superconducting phase with triplet pairing on the T_{cb} line at $x > x_m$ should lead to an abrupt increase in the μSR relaxation rate in a zero external field, as a result of the appearance of internal magnetic fields, which arise because of thorium impurities. This is what was seen experimentally in Ref. 7 at a thorium concentration $\sim 3\%$. The size of the jump corresponds to fields ~ 1 G. Such fields are completely plausible in the volume between thorium impurities. The situation is that anisotropic magnetization distribution (6) in the volume around an impurity falls off in accordance with a power law out to distances less than ξ_0. Superimposed on this power law is an oscillation with a period of $(2k_F)^{-1}$. This circumstance could not lead to a substantial weakening of field[2] (4) in the volume between impurities, the distance between which at $x \approx 3\%$ is only three times the U–U interatomic distance. This hypothesis could be tested by measuring the rate of μSR relaxation of $\sigma_{KT}(T)$ at various concentrations. For example, as the concentration is reduced from $x = 3\%$ to $x_m = 1.7\%$, the jump in $\sigma_{KT}(T)$ should disappear. Furthermore, $\sigma_{KT}(T)$ should increase with decreasing temperature in UBe_{13} with any impurities, not exclusively thorium.

The triplet pairing mechanism, which is required for this explanation of μSR experiments on $U_{1-x}Th_xBe_{13}$, does not contradict measurements[7] of the Knight shift in this substance, according to which there is a significant decrease in this shift in the superconducting state at $x = 0$. This shift gradually fades away with increasing thorium concentration. There is no contradiction here, since the paramagnetic susceptibility in superconductors with a strong spin-orbit coupling decreases with decreasing temperature even in the case of triplet pairing, and the spin-orbit scattering by impurities results in an increase in the susceptibility.

We note in conclusion that the muon experiments[7] were also discussed in another theoretical paper,[11] but the treatment in that paper is difficult to agree with in many regards.

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[1] Since we are talking about a calculation of quantities which are nonzero only to the extent that there is an asymmetry in the distributions of particles and holes near the Fermi surface, we must use the ordinary formalism of superconductivity theory, not the quasiclassical formalism.[6]

[2] The quantity $H_{sp} \propto \mu_B n\, T_c/\varepsilon_F$ in UBe_{13} can be on the order of 10 G.

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