Domain structure and state density in heavy-fermion superconductors

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The spectrum of excitations of a heavy-fermion superconductor at $T = 0$ may contain anomalous branches associated with a domain structure of the superconducting phase. Such a spectrum gives rise to a finite state density $N(0)$. A unit volume of a domain wall corresponds to a state density on the order of the normal density.

The electron component of the heat capacity, $C_e(T)$, in a "heavy-fermion" superconductor (e.g., UBe_{13} or UPt_3) is proportional to T^3 or T^2 at low temperatures, showing that the gap in the excitation spectrum vanishes at certain points (in the case of an axial phase) or on entire lines (a polar phase) on the Fermi surface (see, for example, the review by Moshchalkov and Brandt[1]). Recent studies of C_e in UBe_{13} (Refs. 2–4) and UPt_3 (Refs. 5–7) in the interval 50–300 mK, however, have revealed a linear contribution $C_e = \gamma T + \beta T^{2-3}$, where γ corresponds to a state density $N(0)$ which amounts to $\sim 1\%$–5% of the normal density.

This behavior of $C_e(T)$ can be linked with the presence of impurities, but even in the Born approximation,[8,9] and with resonant scattering,[2,10,11] it has been shown that a certain critical defect concentration is required for the appearance of a nonzero $N(0)$ in an axial superconductor. (Incidentally, it is not clear whether the superconducting phase in UPt_3 is axial, although, even in the polar phase, the critical concentration is zero only in the Born approximation. In the experiments of Refs. 2–7 the defect concentration in the samples was apparently below the critical level. Ott *et al.*,[2] have shown that incorporating resonant scattering leads to a fairly good approximation of the experimental curves if the impurity concentration and the scattering phase shift are chosen appropriately, but in this case there is no linear component in C_e.

In the present letter we wish to propose an alternative explanation of the behavior of $C_e(T)$ in an axial superconductor. The appearance of a nonzero $N(0)$ stems from a domain structure in the superconducting order parameter. We assume that the superconductivity is a triplet superconductivity[12] ($S = 1$)

$$\hat{\Delta}(\mathbf{k}) = i\hat{\sigma}^y(\vec{\hat{\sigma}}\mathbf{d}(\mathbf{k})). \quad (1)$$

The strong spin-orbit coupling in heavy-fermion compounds has the consequence that under rotations of the crystal lattice the vector **d** should transform in accordance with irreducible representations of the point rotation group of the crystal[13]:

$$\mathbf{d}(\mathbf{k}) = \sum_j \sum_i \eta_i^j \vec{\Phi}_i^j(\mathbf{k}), \quad (2)$$

where j is the number of the representation, and i is the number of the basis function $\vec{\Phi}(\mathbf{k})$ in it.

A superconducting phase which grows from nucleating regions that arise independently at T_c will unavoidably have a domain structure in which the coefficients η vary from domain to domain and the transition region (the domain wall) has a thickness on the order of $\xi = v_F/\Delta_0$. We consider the case in which only the two-dimensional coordinate representation is involved in expansion (2) of the superconducting order parameter in a crystal of tetragonal or hexagonal symmetry (for example, UPt_3, $CeCu_2Si_2$, and U_6Fe)

$$d_z = \eta_1 k_x + \eta_2 k_y, \quad d_x = d_y = 0. \tag{3}$$

This form of $\mathbf{d}$ corresponds to an axial superconducting phase.[13]

We assume that η_1 changes sign as we go through a domain wall oriented perpendicular to the x axis, while η_2 remains constant:

$$\eta_1 = (i\Delta_0/2k_F)\tanh(x/\xi), \quad \eta_2 = \Delta_0/2k_F, \tag{4}$$

so that far from the wall we have $d_z = (\Delta_0/2k_F)(\pm ik_x + k_y)$.

We perform a standard canonical transformation of the ψ operators:

$$\psi_{\uparrow(\downarrow)}(\mathbf{r}) = \sum_\nu (u^\nu_{1(2)}(\mathbf{r})a^\nu_{\uparrow(\downarrow)} + \overset{*}{v}{}^\nu_{1(2)}(\mathbf{r})\overset{+}{a}{}^\nu_{\uparrow(\downarrow)}), \tag{5}$$

where the summation runs over all states. The Bogolyubov equations for u and v can be written [we are using Eqs. (1) and (3)]

$$\hat{H}\varphi_1 = (\epsilon\hat{\tau}_3 - \eta_2 k_y \hat{\tau}_1 - i\eta_1 k_x \hat{\tau}_2)\varphi_1 = E\hat{1}\varphi_1, \tag{6}$$

where $\epsilon = -(\nabla^2 + k_F^2)/2m$, $\hat{\tau}_i$ are the Pauli matrices in particle-hole space, and $\varphi_1 = \binom{u_1}{v_2}$; $\varphi_2 = \binom{u_2}{v_1}$ satisfies exactly the same equation. Separating out the dependence on the "good" quantum numbers k_y and k_z, and performing the rotation

$$\varphi_1 \to \exp(i\pi\hat{\tau}_2/4)\tilde{\varphi}\exp(-i(k_y y + k_z z)),$$

where $\tilde{\varphi}(x) = \binom{\tilde{u}(x)}{\tilde{v}(x)}$, we easily find a solution of Eqs. (4) and (6) which is associated with a nonzero state density $N(0)$:

$$\tilde{v}(x) \approx 0, \quad \tilde{u}(x) = \left\{C_1\cos(\alpha x/\xi) + C_2\sin(\alpha x/\xi)\right\}/\cosh(x/\xi), \tag{7}$$

$$E(k_y) = \Delta_0 k_y/k_F. \tag{8}$$

Here $\xi = k_F/m\Delta_0$, $\alpha^2 = \xi^2(k_F^2 - k_y^2 - k_z^2)$, and the coefficients C_1 and $C_2 \sim \xi^{-1/2}$ are determined by the normalization, $\int|\tilde{u}(x)|^2 dx = 1$. The anomalous branches of the type in (8) in the excitation spectrum, which intersect the $E = 0$ level, have already been studied in the superfluid A phase of ^3He (Refs. 14–16). Associated with branch (8) is a state density (per unit surface area of the wall and for the two spin orientations)

$$N_S(0) = \int dk_y\, dk_z\, dx\delta(E)|v|^2/(2\pi)^2 = (k_F/\Delta_0)\int_{-k_F}^{+k_F} dk_z/(2\pi)^2 = k_F^2/2\pi^2\Delta_0, \quad (9)$$

which will be $N_V(0) \sim N_S(0)/\xi = mk_F/2\pi^2$ per unit volume of the wall, i.e., on the same order of magnitude as in a normal metal. The ratio of the state density in the sample to the normal density in this case is on the order of the ratio of the total volume of the domain walls to the volume of the sample.

We will now show that an asymmetric branch of the type in (8), found for wall (4), exists and is unique for a wide class of walls, to which (4) belongs. We assume $\eta_2 = \Delta_0/k_F = \text{const}$ and

$$\eta_1 = \begin{cases} \pm i\eta_2 & \text{for } |x| \gg \xi, \quad (10a) \\ i\eta_2 ax/\xi & \text{for } |x| \ll \xi, \quad (10b) \end{cases}$$

where $a \sim 1$.

Let us find the Atiyah-Singer index I, by substituting (10) into expression (6) for the Hamiltonian $\hat{H}$ and by treating the quantum numbers k_y and k_z as parameters:

$$I(\hat{H}) = \frac{2}{\sqrt{\pi}} \operatorname{tr} \int_0^\infty dy \int dx \sum_n \varphi_n^*(x) \left\{ \hat{H} \exp(-y^2\hat{H}^2) \right\} \varphi_n(x), \quad (11)$$

where φ_i is a complete system of eigenfunctions of $\hat{H}$. [See Ref. 16 for the underlying mathematics and for references on the index theorem. We have omitted from definition (11) the so-called continuous part of I, which is zero for this $\hat{H}$; see also Ref. 16.] Replacing H by E_n in (11) and using the normalization $\int|\varphi_n(x)|^2 dx = 1$, we immediately find $I = \Sigma_n \operatorname{sgn}(E_n)$. In other words, when one of the spectral branches E_k crosses zero, the index I changes by ± 2. Going through the calculations [which are conveniently carried out in momentum space, by taking η_1 as in (10b)], we find

$$I = \operatorname{sgn}(ak_y). \quad (12)$$

The value of I is determined primarily by the region $|x| \leq \xi(\Delta_0/\epsilon_F)^{1/2}$; i.e., linearization (10b) is correct. It follows from (12) that the index I changes by ± 2 as the sign of k_y changes. The spectrum $E(k_y)$ therefore has precisely one asymmetric branch of type (8) which is associated with a state density $N(0)$.

In summary, the presence of a linear term γT in $C_e(T)$ can be associated with walls between superconducting domains. Experiments at $T < 50$ mK may prove decisive for determining whether the distortion of the ordinary behavior $C_e = \beta T^3$ in an axial superconducting phase is associated with impurities or with the superconducting domain walls.

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