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Fulde-Ferrell state in heavy-fermion superconductors

Guimei Yin and Kazumi Maki
Department of Physics, University of Southern California, Los Angeles, California 90089-0484
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Within the weak-coupling model we study the upper critical field of S-wave and D-wave superconductors in the clean limit close to the Chandrasekhar-Clogston limit. We find for parameters derived from $dH_{c2}(T)/dT_{T=T_c}$ of a single crystal of the recently discovered heavy-fermion superconductor UPd_2Al_3 that the Fulde-Ferrell (FF) state is possible for the S-wave and one of the D-wave superconductors of D_{6h} symmetry but not for the hybrid state. Indeed, choosing a g factor slightly less than 2, we can describe the temperature dependence of $H_{c2}(T)$ for both $\mathbf{H}\|\mathbf{c}$ and $\mathbf{H}\|\mathbf{a}$ extremely well. On the other hand the D-wave model predicts the transition into the FF state at $T/T_c=0.29$ in sharp contrast to the experimental observation $T/T_{c0}=0.8$.

A nonuniform superconducting state in the Chandrasekhar-Clogston limit[1,2] in a strong magnetic field has been predicted almost three decades ago by Fulde and Ferrell[3] (FF) and by Larkin and Ovchinnikov.[4] Later this nonuniform state was considered in type-II superconductors by Gruenberg and Gunther.[5] Unfortunately this state requires (a) a system in the clean limit (i.e., $l/\xi \gg 1$ where l is the electron mean free path and ξ is the BCS coherence length) and (b) a large Ginzburg-Landau parameter ($\kappa \gg 1$), which excludes most of the ordinary type-II superconductors.

The appearance of novel superconductors like heavy-fermion superconductors, organic superconductors, and high-T_c copper oxide superconductors in recent years has changed completely this unappealing perspective. Most, if not all, of these novel superconductors satisfy the above two stringent conditions. Therefore it is quite natural to look for a possible FF state where the effect of Pauli limiting is clearly visible. In particular the temperature dependences of the upper critical field $H_{c2}(T)$ in $CeCu_2Si_2$, URu_2Si_2, and UPd_2Al_3 among heavy-fermion superconductors exhibit clearly the effect of the Pauli paramagnetism.[6-9]

In fact Gloos *et al.*[9] found recently a first-order transition curve lying just below the upper critical field of a single crystal of UPd_2Al_3 for both the $\mathbf{H}\|\mathbf{c}$ and $\mathbf{H}\|\mathbf{a}$ configurations. Further, this first-order transition curve terminates at $H_{c2}(T)$ around $T/T_c=0.8$ where T_c is the superconducting transition temperature. Since such a first-order transition is expected[5] between the Fulde-Ferrell state and the usual Abrikosov vortex state, Gloos *et al.* proposed that they saw the FF state in UPd_2Al_3.

In the following we shall study within the weak-coupling model the possibility of the FF state for S-wave and D-wave superconductors. Specifically we shall consider three superconducting states with $f=1$ (S-wave), $\cos\theta\sin\theta e^{\pm i\phi}$ (hybrid) and $\sin^2\theta e^{\pm 2i\phi}$ (D-axial) where f is the wave function associated with the superconducting order parameter in the absence of a magnetic field and (θ,ϕ) is the polar coordinate for the quasiparticle momentum with the polar axis parallel to the c axis. Exact or approximate wave functions of the FF state are constructed by generalizing the standard method used for the ordinary vortex state.[10,11]

As an example we show the coupled integral equations which determine the upper critical field for the D-axial state for $\mathbf{H}\|\mathbf{c}$

$$-\ln t=\int_0^\infty \frac{du}{\sinh u}\int_0^1 dz(1-z^2)^2\{1-e^{-x}(1-2Cx)F(u,z)\}\ , \tag{1}$$

$$-C\ln t=\int_0^\infty \frac{du}{\sinh u}\int_0^1 dz(1-z^2)^2[C-e^{-x}\{\tfrac{1}{6}x^2+C(1-8x+12x^2-\tfrac{16}{3}x^3+\tfrac{2}{3}x^4)\}F(u,z)]\ , \tag{2}$$

where

$$F(u,z)=\cos(\alpha B u/t)\cos(\alpha B\tilde{q}uz/t)\ ,$$
$$\alpha=g\mu_B/2\pi T_c=0.058\,74g/\text{Tesla}, \tag{3}$$
$$x=\alpha_1 B t^{-2}u^2(1-z^2)\ ,\quad z=\cos\theta,\quad t=T/T_c$$

and $\alpha_1=2v_1^2e/(2\pi T_c)^2$ and the solution of Eqs. (1) and (2) is identified $B=H_{c2}(t)$. Here $\tilde{q}=v(q/g\mu_B B)$ and the FF state corresponds to the one with $\tilde{q}\neq 0$. α_1 is a parameter describing the orbital effect and determined from $dH_{c2}(T)/dT_{T=T_c}$. For the D-axial state and for $\mathbf{H}\|\mathbf{c}$ we obtain

$$\alpha_1=0.04/\text{Tesla}\ , \tag{4}$$

which corresponds to $dH_{c2}(T)/dT_{T=T_c}=-3.75$ Tesla/K and $T_c=1.8$ K. Therefore if we choose $g=2$, there will be no adjustable parameter within the present theory. Equations (1) and (2) are obtained by taking the ground state given by[11]

$$\Phi=\sin^2\theta\{e^{-2i\phi}+Ce^{2i\phi}(a^+)^4\}e^{iq\cos\theta z}|0\rangle\ , \tag{5}$$

where $|0\rangle$ is an Abrikosov-like wave function consisting of the linear superposition of the lowest Landau-level wave functions, a^+ is the raising operator, and C is a constant depending on t and $\tilde{q}$. We note in passing that when $\mathbf{H}\|\mathbf{a}$ the wave function of the D-axial state changes into

$$\Phi=(3\cos^2\theta-1)e^{iq\cos\theta x}|0\rangle\ , \tag{6}$$

where now we took the polar axis along the a axis.

In Figs. 1 and 2 we show the upper critical field determined in this way for three states ($f=1$, $f=\sin\theta\cos\theta e^{-i\phi}$, and $f=\sin^2\theta e^{-2i\phi}$), without the Pauli term ($g=0$) and $g=2$ for $\mathbf{H}\|\mathbf{c}$ and $\mathbf{H}\|\mathbf{a}$, respectively. Also included in Fig. 1 is the upper critical field of the octahedral state ($f=\frac{1}{2}[(3\cos^2\theta-1)+i\sqrt{3}\sin^2\theta\cos(2\phi)]$), since this state has only point zeros and gives a T^3 specific heat consistent with observation. However, this state does not have D_{6h} symmetry. When $\mathbf{H}\|\mathbf{a}$ the octahedral state gives the same upper critical field as the D-axial state. Also we show in these figures curves of $H_{c2}(T)$ due to the Pauli term only, which is independent of the wave function f and the field orientation. If α_1 determined from the slope of the upper critical field at $T=T_c$ (see Table I for a list) is used, we find that the observed upper critical field lies between the two curves ($g=0$ and $g=2$) for all three states. Further we find that the FF state is not possible for the hybrid state but the FF state gives the highest $H_{c2}(T)$ for both the S-wave and the D-axial state, though for the S-wave state the difference in $H_{c2}(T)$'s for the FF state and the $q=0$ state is only a few percent (see Table I). The theoretical curves can be brought closer to those observed by reducing the g factor. Indeed by choosing g somewhat smaller than 2, we obtain excellent fits as shown in Figs. 1 and 2. However, for this reduced g value the FF state survives only for the D-axial and the octahedral state. Again we list

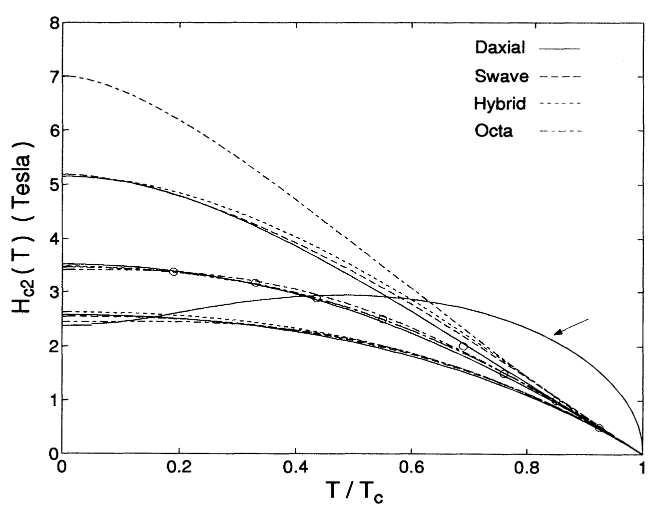

FIG. 1. The upper critical field for D-axial (——), S (— — —), hybrid (· · · ·), and octahedral (—·—·—·) state for $\mathbf{H}\|\mathbf{c}$ are shown for $g=0$ (no Pauli term), $g\cong1.18$, and $g=2$ from top to bottom. The open circles are experimental values taken from Gloos *et al.* (Ref. 9). Also the solid curve with arrow is the one in the pure Pauli limit (no orbital effect). The best fit to experimental data is obtained for $g\cong1.18$. However, for this g value there is no FF state even for the D-axial state, which is most favorable.

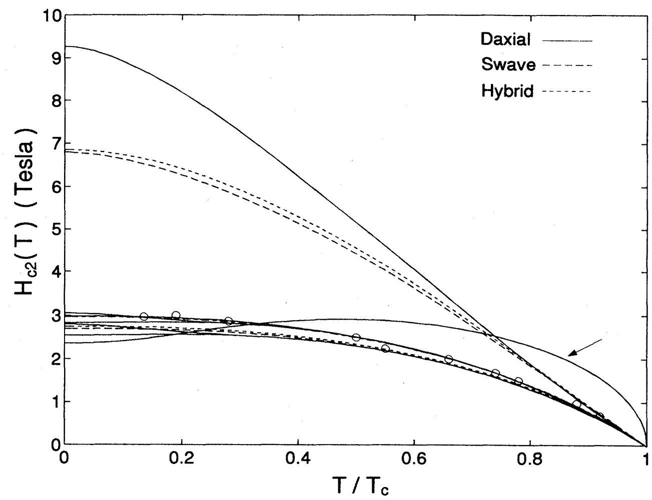

FIG. 2. The upper critical field for the D-axial (——), S (— — —), and hybrid (· · · ·) state for $\mathbf{H}\|\mathbf{a}$ are shown for $g=0$, $g\cong1.76$, and $g=2$ from top to bottom. Two curves for the D-axial state are for the FF state (upper one) and the ordinary $q=0$ state. Open circles are taken from Ref. 9. Even for the most favorable case (D axial) the FF state terminates at $T/T_c=0.29$.

TABLE I. Summary of the pertinent parameters in our calculation. The second column is the field direction, α_1 controls the orbital effect, $\tilde{q}$ is the dimensionless q vector characterizing the FF state at $T=0$ K, and $h_{\rm FF}$ is the ratio of H_{c2} associated with the FF state and the $\tilde{q}=0$ state at $T=0$ K. Finally $t_c=T/T_c$ where the FF state terminates. Even in the most favorable case (D-axial state) the FF state terminates at $T/T_c=0.29$. There is no FF state for the hybrid state.

State		α_1 (Tesla)$^{-1}$	g	$\tilde{q}$	$h_{\rm FF}$	t_c
S wave	a	0.038	2	0.85	1.01613	0.3
			1.76	0.71	1.00881	0.26
	c	0.05	2	0.57	1.0026	0.15
			1.18	0	0	0
D axial	a	0.058	2	0.94	1.10071	0.34
			1.76	0.92	1.07797	0.29
	c	0.04	2	0.31	1.0097	0.6
			1.18	0	0	0
Hybrid	a	0.05	2	0		
			1.82			
	c	0.11194	2	0		
			1.26			

the corresponding g values in Table I. Therefore we can describe the observed upper critical field with a very simple model. Perhaps an anisotropy in the g factor required for this fit may be a little too large. However, there is a serious difficulty in identifying the observed $H_{c2}(T)$ for the FF state for the S-wave or the D-wave state. First of all, for this reduced g factor the FF state disappears completely when $\mathbf{H}\|\mathbf{a}$. Further, the present model predicts that even in the most favorable case (D-axial case) and $\mathbf{H}\|\mathbf{c}$ the FF state terminates at $T/T_c=0.29$ in contrast to $T/T_c=0.8$ as observed experimentally. At lower temperatures the FF state is most favorable for the D-axial state for $\mathbf{H}\|\mathbf{c}$, if the effect of the impurity scattering is neglected. Therefore in order to establish definitively the presence of the FF state a few things have to be done. From the theoretical point of view the role of spin-orbit coupling and impurity scattering has to be clarified. Also it is possible the weak antiferromagnetism present in UPd_2Al_3 may change the stability region of the FF state and the phase diagram as in UPt_3. In particular, if the antiferromagnetism had a long-range (~ 100 Å) modulation, it would help to stabilize the FF state. In any case, understanding the nature of the first-order transition in the vortex state is the most urgent in order to clarify the nature of the superconductivity in UPd_2Al_3.

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