Modulated vortex lattice in high fields and gap nodes

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The mean field vortex phase diagram of a quasi-two-dimensional superconductor with a nodal d-wave pairing and with strong Pauli spin depairing is studied in the parallel field case in order to examine the effect of gap nodes on the stability of a Fulde-Ferrell-Larkin-Ovchinnikov- (FFLO-) like vortex lattice. We find through a heuristic argument and a model calculation with a fourfold anisotropic Fermi surface that the FFLO-like state is relatively suppressed as a field approaches a nodal direction. When taking account of available experimental results together, the present result strongly suggests that the pairing symmetry of CeCoIn5 should be of d_u type.

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In a recent paper1 (denoted as I hereafter), we examined the vortex phase diagram of quasi-two-dimensional (Q2D) type II superconductors with strong Pauli paramagnetic (spin) depairing by focusing on the H//c case with a field H perpendicular to the superconducting layers. In contrast to earlier work2,3 taking account of both the orbital and spin depairing effects of the magnetic field in the clean limit, the orbital depairing was incorporated fully and nonperturbatively there,1 and two results opposite to those suggested previously2,3 were found. First of all, the mean field (MF) transition at the H_c2(T) line changes from the familiar second-order one to a first-order (MF-FOT) one4–6 at a higher temperature T' rather than the region in which a Fulde-Ferrell-Larkin-Ovchinnikov- (FFLO-) like7,8 modulated vortex lattice may appear. This feature is consistent with data for CeCoIn5 in H//c.5–7,9 Second, a second-order transition curve HFLO(T) between such a FFLO-like and ordinary vortex lattices remarkably decreases upon cooling. Interestingly, these two results are also consistent with more recent data for CeCoIn5, suggesting a structural transition to a FFLO state, in H//c.9–12 A recent ultrasound measurement11 also shows that the suggested FFLO state is, as we argued in I, a kind of vortex lattice. However, it should be further examined theoretically whether this qualitative agreement with the data in H//c is justified or not.

In this paper, the results of the application of the analysis in I to a model for the H//c case are reported. By including the contributions, neglected in previous work1–3 from the non-Gaussian (|Δ(r)|^4 and |Δ(r)|^6 terms of the Ginzburg-Landau (GL) free energy to the spatial gradient parallel to H, where Δ(r) is the pair field, we find that the relative position between T' and the HFLO line is qualitatively the same as in the H//c case1 as long as a spin depairing strength realistic in bulk superconductors is used; and that, at least close to HFLO, the LO state3,8 with periodic nodal planes perpendicular to H of |Δ| is more stable than the FF state3,7 composed of a phase modulation keeping |Δ| fixed.

Special attention is paid in this paper to the noticeable in-plane angular dependence of the FFLO curve HFLO(T) found in specific heat9 and magnetization12 data for CeCoIn5: The observed FFLO curve in H//||110|| lies at higher temperatures than that in H//||100||. This HFLO anisotropy is much more remarkable9 than that of H_c2(T) and may give decisive information about the fourfold anisotropy of the gap function. As long as the in-plane Fermi velocity anisotropy is negligible, it is heuristically predicted by the following simple argument that a gap anisotropy results in a HFLO anisotropy: Near the gap nodes where the superconducting gap Δ_k is small, the coherence length ξ_0 ≈ ℏv_F/Δ_k defined locally in the k space is longer.13 The orbital limiting field H_2(0) is inversely proportional to the square of the averaged coherence length in the plane perpendicular to H and hence is minimal when H is directed along the fourfold symmetric gap nodes (or minima). Since a higher H_2eb will lead to a relatively stronger effect of spin depairing, the FFLO curve and T', induced by the spin depairing, are expected to lie at higher temperatures when H is located along a gap maximum. If we compare the expected HFLO anisotropy with the observations9,12 in CeCoIn5, we inevitably reach the conclusion that, in agreement not with the original argument4 favoring a d_u,xy pairing just as in high-Tc cuprates but with a recent report on low-H specific heat data,14 a node (or minimum) of the gap function of CeCoIn5 is located along the [100] direction, implying a d_u,xy pairing state. Below, we will show how this conclusion is reinforced through a microscopic derivation of HFLO(T) taking account of a possible in-plane fourfold anisotropy of the Fermi surface (FS). The present result might require a serious change in the picture of the pairing mechanism of CeCoIn5 based upon similarities of the normal state properties, including the presence of antiferromagnetic fluctuation, to the high-Tc cuprates.15

First, let us sketch an outline of the MF analysis1 for H//c. Throughout this paper, we assume H=H± and the d-wave gap function w_± = ±(1/2) cos(2φ) or ±(1/2) sin(2φ), where φ is the azimuthal angle in the a-b plane. Within the lowest (N=0) Landau level (LL), the GL free energy density in the MF approximation takes the form

\[ F = \int d^3r \left[ \frac{1}{2m} \left( \nabla \phi - A \right)^2 + \frac{\lambda}{4} \phi^4 \right] + \frac{\alpha}{2} \left( \nabla \phi \right)^2 \]

where \( \phi \) is the order parameter, \( A \) is the gauge field, \( \lambda \) is the coupling constant, and \( \alpha \) is the pair-breaking parameter. The MF equations are obtained by minimizing \( F \) with respect to \( \phi \) and \( A \). In the MF approximation, the order parameter is given by the solution of the following equation:

\[ \nabla^2 \phi = 2 \lambda \phi^3 - \alpha \nabla^2 \phi \]

The solutions of this equation are determined by the boundary conditions at the Fermi surface. For example, in the case of a two-dimensional superconductor, the solutions are given by:

\[ \phi(r) = \frac{\lambda}{\alpha} \left( 1 - \frac{r^2}{\xi^2} \right) \]

where \( \xi \) is the coherence length. In the case of a three-dimensional superconductor, the solutions are given by:

\[ \phi(r) = \frac{\lambda}{\alpha} \left( 1 - \frac{r^2}{\xi^2} \right)^{1/2} \]

These solutions are valid only for small values of \( r \). For large values of \( r \), the order parameter is given by the solution of the following equation:

\[ \nabla^2 \phi = 2 \lambda \phi^3 - \alpha \nabla^2 \phi \]

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The essential part of the MF analysis in I is to derive the coefficients, $a_0$, $V_d$, $V_0$, $c_2$, and $c_4$ by starting from the weak-coupling BCS model with a Zeeman (Pauli paramagnetic) term. Here, $N(0)$ is the averaged density of states (DOS) at the Fermi level, and $\langle \rangle$ is the spatial average on $x$ and $z$.

The extension of $\Delta(r)$ was expanded in terms of the LLs as $\Delta(r) \equiv \sum_{N=0}^{\infty} \Delta_Q^{(N)}(y,z)u_Q(x)$, and the higher LLs were neglected above. For the LO (FF) state, $u_Q(x)$ takes the form $\cos(Qx) \exp[iQx]$. A Q2D FS with a circular form in the $y$-$z$ plane was assumed, although in-plane anisotropy will conveniently be included as the $\phi$ dependence of the Fermi velocity and DOS [see Eq. (5) below]. For an example, $a_0(Q)$ is, after performing the $k$ integrals and introducing a parameter integral, expressed by

$$
F_{MF} = N(0) \left[ a_0(Q)\langle\Delta_Q^{(0)}\rangle^2 + \frac{V_d(Q)}{2} \langle\Delta_Q^{(0)}\rangle^4 \right] + \frac{V_0(Q)}{3} \langle\Delta_Q^{(0)}\rangle^6
$$

$$
= c_0 + c_2 Q^2 + c_4 Q^4.
$$

(1)

The specific heat anomaly 9 in CeCoIn$_5$ in $H||c$ at low enough temperatures may be rather due to a transition between straight vortex lattices in the $N=0$ and $N=1$ LLs. A detailed study of this transition into an $N=1$ LL state will be reported elsewhere.

Now, let us turn to the $H \perp c$ case. Although, in principle, the above analysis can be extended to a Q2D system with a cylindrical FS under $H$ perpendicular to the cylindrical axis, we have chosen to work in an elliptic FS elongated along the $z(||c)$ axis and with the dispersion relation $e_k = h^2 \Sigma_{N=2} \gamma N_k^2/(2m)$ under $H||c$ in order to make numerical calculations more tractable, where $\gamma_1 = \gamma_2 = \gamma^{1/2}$, and $\gamma_2 = \gamma$ with $\gamma \geq 1$ and a constant $\tilde{m}$. We expect the case with a moderately large $\gamma$ value to qualitatively describe essential features in the realistic Q2D case. By isotropizing the $k$ vector as $k = \gamma k_F \hat{r}$, where $\hat{r} = (\cos \phi \sin \theta, \sin \phi \sin \theta, \cos \theta)$ is the unit vector in spherical coordinates, the velocity $v$ on the FS is written as $v_j = \gamma v_F \hat{r}_j$. The Jacobian $\sqrt{\gamma} \sin \phi \sin \theta + \gamma^2 \cos^2 \theta$ accompanying the angular integral along the FS is exactly canceled by the angular dependence of the DOS, $N(\theta) = \gamma N(\phi) / \Sigma_j v_j^2$. Again, the in-plane (four-fold) anisotropy of the FS will first be neglected. Then, the GL free energy within the $N=0$ LLs takes the form of Eq. (1), and the function $g^{(0)}(\rho, -i\phi_2)$ appearing in $a_0(Q)$ [see Eq. (3)] is replaced in the present case by

$$
g^{(0)}_\parallel(\rho, -i\phi_2) = \int_0^{2\pi} \frac{d\theta}{4\pi} N(0)|w_{\phi_2}|^2 \exp(-\rho^2 v_{\phi_2}^2/4\gamma_2) \times \cos(-i\rho v_{\phi_2} \phi_2.,
$$

where $v_{\phi_2}^2 = \eta^2 v_2^2 + \eta \tilde{v}_2^2$. The parameter $\tilde{\eta}$ is insensitive to the uniaxial anisotropy $\gamma$ but dependent on $T$ and needs to be determined by maximizing $H(2)(T)$. By focusing on the low-$T$ region, we find that $\tilde{\eta}$ takes a value between 0.4 and 0.5 depending on the relative angle between $H$ and the nearest nodal direction. Using this parameter, the anisotropy in spatial variations of $\Delta(r)$ within the $y$-$z$ plane is given by $\gamma/\tilde{\eta}$. Except for the modifications indicated above, the corresponding quartic and sixth-order terms of the GL free energy are derived by closely following the analysis in I. We choose $a_0 = \mu_0 H_{\phi_2}^{\gamma=1}(0)/k_B T_0$ as a measure of the spin dephasing strength in $H \perp c$, where $H_{\phi_2}^{\gamma=1}(0)$ is the orbital limiting field in the isotropic case.

In Fig. 1, the resulting phase diagram is shown to illustrate how the $H_{\phi_2}(T)$ position depends upon the relative angle between $H$ and the nodal directions. Thin solid (chain) curves are defined by $a_N(0)=0$, and the $H(2)(T)$ in $T>T'$ in each case is given by each $a_0(0)=0$ line. In agreement with the heuristic argument given earlier, $H(2)(T)$ and $T'$ are shifted to higher temperatures as the in-plane field is directed along a gap maximum, reflecting an enhanced spin dephasing.
in this field configuration. As in $H_{\|c}$, the FFLO state at least close to $H_{\text{FFLO}}$ has the LO-like variation. By combining our numerical calculations with an analytical calculation with the orbital depairing perturbatively included, we have verified that such an in-plane $H_{\text{FFLO}}$ anisotropy is absent without the orbital depairing (i.e., when $a_s(0) = 0$) and monotonically increases with decreasing $a_s$. In contrast, it is not easy to properly predict the corresponding anisotropy (in-plane angular dependence) of the $H_{c2}(T)$ curve. First, the depression of $H_{c2}$ due to the spin depairing is larger as the corresponding $H_{c2}(0)$ is higher, and hence the $H_{c2}$ magnitude may not have a monotonic $a_s$ dependence. Second, the MF-FOT line of $H_{c2}$ is directly determined by the details of the non-Gaussian terms other than the quartic one in the GL free energy and hence is quantitatively affected by our assumption of keeping the non-Gaussian terms only up to $|\Delta|^6$ in Eq. (1). Actually, the rapid increase of the MF-FOT line on cooling *just* below $T^*$ arises due to an extremely small $V_d(0)$ near $T^*$ and might flatten if we could numerically include the $|\Delta|^8$ and higher-order terms. In contrast, the $V_6$ contribution to $c_2$ [i.e., to $H_{\text{FFLO}}(T)$] was negligible, as in the $H_{\|c}$ case, consistent with the smallness of $V_d(0)$ mentioned above. We expect that the $H_{\text{FFLO}}(T)$ curve is less sensitive to the neglect of the $|\Delta|^8$ and higher-order GL terms. For these reasons, we will focus hereafter on $T^*$ and $H_{\text{FFLO}}$ which directly measure the (effective) spin depairing strength. The resulting anisotropies of $T^*$ and $H_{\text{FFLO}}$ in Fig. 1 qualitatively agree with those of CeCoIn$_5$ in $\gamma\beta\hat{k}$ if a gap node (or minimum) is located along [100]. As already mentioned, the MF-FOT line in the $N=0$ LL needs to lie above the corresponding $a_j(0)=0$ line in order for $H_{\text{FFLO}}(T)$ to be realized as a transition line. As Fig. 1 shows, this condition manages to be satisfied, in contrast to the $H_{\|c}$ case.

In order to examine how the result in Fig. 1 is affected by the in-plane FS anisotropy, let us next introduce it as a Fermi velocity anisotropy in a similar manner to Ref. 16:

\begin{equation}
\nu_f \rightarrow \nu_f(\phi) = \nu_f[1 + \beta \cos(4\phi)],
\end{equation}

where $|\beta|<1$, accompanied by the replacement $N(0) \rightarrow N(0)\nu_f/\nu_f(\phi)$ in any angular integral [see Eq. (4)]. Apart from these replacements in our calculation, the derivation of phase diagrams is quite the same as that of Fig. 1. When $\beta>0(<0)$, the Fermi velocity becomes maximal (minimal) along $\phi$. By combining these two cases with the two candidates $\sqrt{2}\cos(2\phi)$ and $\sqrt{2}\sin(2\phi)$ for $\nu_f$, we have four different cases of the relative anisotropies under a fixed $H_{\|c}$. We will classify them into two categories, (a) $\nu_f = \sqrt{2}\cos(2\phi)$ with $\beta<0$ and $\nu_f = \sqrt{2}\sin(2\phi)$ with $\beta>0$, and (b) $\nu_f = \sqrt{2}\cos(2\phi)$ with $\beta>0$ and $\nu_f = \sqrt{2}\sin(2\phi)$ with $\beta<0$. This classification is motivated by the result\textsuperscript{16} that, in the category (a), the Fermi velocity anisotropy and the pairing anisotropy favor different orientations, competing with each other, of the square vortex lattices to be realized in fourfold anisotropic $d$-wave superconductors in $H_{\|c}$, while such a competition does not occur in (b). In Fig. 2, the resulting phase diagrams for the categories (a) and (b) are given. In the case (a), the angular dependences of $H_{\text{FFLO}}$ and $T^*$ are weakened by the FS anisotropy compared with those in Fig. 1, while the opposite tendency is seen in the case (b). This result can be understood by noting that the orbital depairing strength locally in the $\mathbf{k}$ space is measured in the
present case by \(v_z^2\) in Eq. (4) (note that, in the 2D limit, \(v_z^2\) is absent there). By focusing on the case with \(H\) parallel to a gap node and noting \(|\omega_d|^2\) in the integrand of Eq. (4), one will notice that a nonzero \(\beta\) tends to increase (decrease) the contributions of \(v_z^2\), on average, when \(\beta < 0 (\beta > 0)\). Thus, an enhanced orbital depairing in \(H\) parallel to a node of case (b) additionally reduces \(H_{\text{FFLO}}\) so that the difference between the two cases in Fig. 2 follows. Bearing in mind the general character of this interpretation, we believe that the results in Fig. 2 would not be qualitatively changed by a refinement of the microscopic description.

The above results commonly show an \(H_{\text{FFLO}}(T)\) line shifting to higher temperatures as the in-plane field approaches a gap maximum and, compared with the data for CeCoIn\(_3\), imply a \(d_{xy}\) state as the pairing state of this material. Although one might consider the possibility of \(d_{z^2-r^2}\) pairing based on the fact that an extremely strong FS anisotropy in the microscopic description. Al-

12. T. Tayama (private communication).