Vortex state in double transition superconductors

Yasushi Matsunaga,† Masanori Ichioka,‡ and Kazushige Machida

Department of Physics, Okayama University, Okayama 700-8530, Japan

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Novel vortex phase and nature of double transition field are investigated by two-component Ginzburg-Landau theory in a situation where fourfold-twofold symmetric superconducting double transition occurs. The deformation from 60° triangular vortex lattice and a possibility of the vortex sheet structure are discussed. In the presence of the gradient coupling, the transition changes to a crossover at finite field. These characters are important to identify the multiple superconducting phase in PrOs$_4$Sb$_{12}$.

In the newly discovered superconductor PrOs$_4$Sb$_{12}$, which is a heavy-fermion compound with filled skutterudite structure, a novel pairing mechanism is considered in connection to quadrupole fluctuations. Several experimental results suggest unconventional pairing symmetry. In the nuclear spin-lattice relaxation experiment, the coherence peak is absent below the transition temperature. In the magnetic field rotated in the ab-plane of the crystal axes reveals the phase diagram of the double transition, and shows that a fourfold-symmetric pairing function around the c-axis in the high-field H-phase is changed to a twofold-symmetric one in the low-field L-phase at the second transition field $H^*$. The relative momentum $(\mathbf{m}, \mathbf{j})$ of the pair is mapped on $\phi^*(\mathbf{r}, \mathbf{k}) = \eta_1(\mathbf{r})\phi_1(\mathbf{k}) + \eta_2(\mathbf{r})\phi_2(\mathbf{k})$ with the order parameter $\eta_m(\mathbf{r})$, where $\mathbf{r}$ is the center of mass coordinate of the Cooper pair and $m = 1, 2$. The relative momentum $\mathbf{k}$ of the pair is mapped on the Fermi surface. The pairing function is given by $\phi_m(\mathbf{k}) = i\sigma_y \phi_m(\mathbf{k})$ for the singlet pairing, and $\phi_m(\mathbf{k}) = \sum_{j=x,y,z} d_{m,j}(\mathbf{k})\sigma_j \sigma_y$ for the triplet pairing with Pauli matrices $\sigma_x, \sigma_y, \sigma_z$. We assume that the superconducting gap by $\phi_1(\mathbf{k}) (\phi_2(\mathbf{k}))$ has fourfold (twofold) symmetry, and that the transition temperature estimated from the pairing interaction is lower for the second component, i.e., $T_c = T_{c1} > T_{c2}$. Since the pairing symmetry for PrOs$_4$Sb$_{12}$ is not established yet, the pairing function forms $\phi_m(\mathbf{k})$ are not specified in this study.

Within the GL approximation, the free energy in the superconducting state is generally given by $F_s = F_n + \int f(\mathbf{r})d\mathbf{r}$ with

$$f(\mathbf{r}) = -\alpha_0(T_c - T)|\eta_1|^2 - \alpha_0(T_{c2} - T)|\eta_2|^2 + |A_2| \left\{ \frac{1}{2} \text{tr}(\hat{\Delta}^\dagger (\mathbf{v} \cdot \mathbf{q})^2 \hat{\Delta}) + \frac{1}{2} \text{tr}(\hat{\Delta}^\dagger \hat{\Delta}^\dagger \hat{\Delta}) \right\}$$

in the clean limit $\Theta$, where $\mathbf{q} = (\hbar/j)\nabla + (2\pi/\phi_0)\mathbf{A}$, $F_n$ is the free energy in the normal state, $|A_2| = 7\zeta(3)/(16\pi^2T_c^2)$ with Riemann’s $\zeta$-function, $\phi_0$ is a flux quantum, $\mathbf{v}$ is a Fermi velocity, $\cdots$ indicates the Fermi surface average of $\mathbf{k}$, and $\mathbf{A}$ is a vector potential. Since the magnetic field is applied along the z-axis, $q_z = 0$. 



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In the dimensionless form, Eq. (1) is written as

\[ \tilde{f} = \frac{f_0}{\eta_0} = - \left( 1 - \frac{T}{T_c} \right) |\eta_1|^2 - \left( \frac{T_{c2}}{T_c} - \frac{T}{T_c} \right) |\eta_2|^2 + \eta_1^* (q_{x2} + q_{y2}) \eta_1 + C_{22x} q_{y2}^2 \eta_2 + C_{22y} q_{x2}^2 \eta_2 + C_{12x} q_{x2} q_{y2} \eta_1 + C_{12y} q_{x2}^2 \eta_2 + C_{12y}^* q_{y2}^2 \eta_2 + \frac{1}{2} |\eta_1|^4 + C_2 |\eta_2|^4 + 4C_3 |\eta_1|^2 |\eta_2|^2 + C_4 \eta_1^* q_{x2}^2 \eta_2 + C_4 q_{y2}^2 \eta_1^* \eta_2, \tag{2} \]

using \( f_0 = \alpha_0 T_{c2} \), \( \eta_0^2 = \alpha_0 T_c / (2|A_2|C_1) \equiv 1 \) and \( \xi^2 = |A_2|C_{11x} / (\alpha_0 T_c) \equiv 1 \). The coefficients of the gradient terms in Eq. (2) are given by

\[ C_{11x} = \frac{\langle |\phi|^2 |\psi_y^2 \rangle}{\langle |\phi|^4 \rangle}, \quad C_{22x} = \frac{\langle |\phi|^2 |\psi_y^2 \rangle}{C_{11x}} = (1 - c) / \langle X \rangle \sqrt{1 - c^2}, \quad C_{22y} = \frac{\langle |\phi|^2 |\psi_y^2 \rangle}{C_{11x}} = (1 + c) / \langle X \rangle \sqrt{1 - c^2}, \quad C_{12x} = \frac{\langle \phi | \phi_y^2 | \phi \rangle_{\eta_1}}{C_{11x}}, \quad C_{12y} = \frac{\langle \phi | \phi_y^2 | \phi \rangle_{\eta_2}}{C_{11x}}, \tag{3} \]

where \( \phi_m^* \phi_n = \phi_m^* \phi_n \) for the singlet pairing, \( \phi_m^* \phi_n \) for the triplet pairing, and \( \phi_m^* \phi_n \) for the Fermi surface anisotropy parameter \( c \) is not zero since \( \langle |\phi|^2 |\psi_y^2 \rangle \neq \langle |\phi|^2 |\psi_y^2 \rangle \). \( C_{12x} \) and \( C_{12y} \) reflect the strength of the gradient coupling between \( \eta_1 \) and \( \eta_2 \).

The coefficients of the quadratic terms in Eq. (2) are given by

\[ C_1 = \langle |\phi|^4 \rangle, \quad C_2 = \langle |\phi|^4 \rangle / C_1, \quad C_3 = \langle |\phi|^2 |\phi|^2 \rangle / C_1, \quad C_4 = \langle |\phi|^2 |\phi|^2 \rangle / C_1 \] for the singlet pairing, and

\[ C_1 = 2 |d_1|^2 - |d_1|^2, \quad C_2 = 2 |d_2|^2 - |d_2|^2, \quad C_3 = 2 |d_1|^2 |d_2|^2 - |d_1|^2 |d_2|^2, \quad C_4 = 2 |d_1|^2 |d_2|^2 - |d_1|^2 |d_2|^2 / C_1 \] for the triplet pairing. However, we can not identify the definitive values of coefficients in Eq. (2) for PrOs4Sb12, because the detailed information of the pairing function and Fermi surface structure have not been established yet. It is noted that the Fermi surface anisotropy also largely affects on the coefficients. Therefore, we treat these coefficients as arbitrary parameters, and report some typical results obtained in this framework.

Before considering vortex states, we study a uniform state at a zero field. From the free energy minimum condition, the relative phase of \( \eta_1 \) and \( \eta_2 \) becomes \((\alpha + \pi)/2\) with \( \alpha \) given by \( C_1 = |C_4| e^{i\alpha} \). For the H-phase, \( \eta_1 = (1 - T/T_c)^{1/2} \) and \( \eta_2 = 0 \). The second component \( \eta_2 \) appears at the lower transition temperature \( T^* \) given by

\[ T^* = T_{c2} / T_c - (2C_3 - |C_4|) / (1 - (2C_3 - |C_4|)). \tag{4} \]

which is derived by linearizing the equation \( \partial \tilde{f} / \partial \eta_2^* = 0 \). In the presence of \( \eta_1 \), \( T^* \) is suppressed compared with \( T_{c2} \). To assure that \( T^* > 0 \), we have to satisfy \( 2C_3 - |C_4| < T_{c2} / T_c \).

The vortex structure is calculated by the time-evolution following the TDGL equation coupled with Maxwell equation \[ 16, 17 \]

\[ \frac{\partial}{\partial t} \eta_1 = - \frac{1}{12} \frac{\partial \tilde{f}}{\partial \eta_1}, \quad \frac{\partial}{\partial t} \eta_2 = - \frac{1}{12} \frac{\partial \tilde{f}}{\partial \eta_2}, \tag{5} \]

\[ \frac{\partial}{\partial t} A = - \kappa^2 \nabla \times B, \quad B = \nabla \times A. \tag{6} \]

The supercurrent \( \tilde{j}_s = (j_{s,x}, j_{s,y}) \propto (\partial \tilde{f} / \partial A_x, \partial \tilde{f} / \partial A_y) \) is given by

\[ j_{s,x} = \Re[\eta_1^* (q_x \eta_1) + C_{22x} q_x \eta_2 + C_{12x} q_x \eta_1 \eta_2], \tag{7} \]

\[ j_{s,y} = \Re[\eta_1^* (q_y \eta_1) + C_{22y} q_y \eta_2 + C_{12y} q_y \eta_1 \eta_2]. \tag{8} \]

We use the same scale units as in Refs. \[ 16 \] and \[ 17 \] for length, field, and time, except for the order parameters. We here scale \( \eta_m \) by \( \eta_0 \) instead of \( \eta_0(T) = \eta_0(1 - T/T_c)^{1/2} \). In our calculations, we typically use the GL parameter \( \kappa = 4 \), which belongs to a high-\( \kappa \) case, i.e., the order parameter structure is not significantly affected by the internal field distribution.

Calculations are performed in a two-dimensional square area. Outside the open boundary, we set \( \eta_1 = \eta_2 = 0 \) and \( B(\mathbf{r}) = H \) with an applied field \( H \). For the initial state of \( \eta_1, \eta_2 \) and \( A \) inside, we use a uniform state at a zero-field. Through the time evolution, vortices penetrate from the boundary. After enough time later, the time-evolution converges and the vortex lattice state is obtained. We analyze this final state.

![FIG. 1: (a) Maximum of \( |\eta_2(\mathbf{r})| \) (solid lines) as a function of \( H/H_c(0) \). \( T/T_c = 0.1(\times), 0.4(\bullet) \) and 0.7(\( \Delta \)). \( \eta_2 \) appears at \( H < H^* \). For \( T/T_c = 0.1 \). \( H \)-dependence of \( |\eta_1| \) is also presented (a dashed line). (b) \( H-T \) phase diagram in this GL theory. The transition field \( H^* \) and \( H_{c2} \) are presented.](image)
shown in Figs. 2(b) and 2(c). Vortex core shape of near the boundary in the integration over $r$ tex core shapes of (3), coming from the twofold symmetry of $\hat{\eta}$. These peaks are on an ellipse with long axis $2q_x$ and short axis $2q_y$ with the ratio $q_x/q_y \sim 1.2$. For a reference, we also show the diffraction pattern of the $60^\circ$ triangular lattice in the H-phase in Fig. 2(e), where peaks appear on a circle. The observation of this vortex lattice deformation may be another means to detect the fourfold-twofold transition in the $H$-$T$ phase diagram.

![FIG. 2](image)

FIG. 2: (a) Density plot of an internal field distribution $B(r)$ at $H/H_c(0) = 0.2$ and $T/T_c = 0.1$. White region corresponds to the vortex core with large $B(r)$. Density plot of $|\eta_1(r)|$ (b) and $|\eta_2(r)|$ (c) around a vortex. Diffraction pattern $|B_0|^2$ at $H/H_c(0) = 0.2$ (d) and 0.5 [H-phase] (e).

At $H/H_c(0) = 0.2$ and $T/T_c = 0.1$, the vortex distribution is shown in Fig. 2(a), where the internal field distribution is shown as a density plot. There are some domains of the different orientation of the triangular lattice, since the vortex lattice configuration is affected by the boundary. And the triangular lattice is deformed from $60^\circ$ triangle by the effect of finite $c$ in Eq. 3, coming from the twofold symmetry of $\hat{\phi}$. The vortex core shape of $|\eta_1(r)|$ and $|\eta_2(r)|$ are, respectively, shown in Figs. 2(b) and 2(c). Vortex core shape of $|\eta_2(r)|$ is stretched out toward the $y$-direction, while that of $|\eta_1(r)|$ remains to be circular. The deformation of the vortex lattice is clear, when we see the form factor of the internal field distribution, as in the neutron scattering experiments. Figure 2(d) shows the “diffraction pattern” $|B_0|^2$ in the L-phase, with the Fourier component $B_0 = \sum_r e^{i\mathbf{q}\cdot\mathbf{r}}B(r)$, where we exclude the region near the boundary in the integration over $r$. There appear six peaks of the triangular lattice, and the rotated ones for different orientations. These peaks are on an ellipse with long axis $2q_x$ and short axis $2q_y$ with the ratio $q_x/q_y \sim 1.2$. For a reference, we also show the diffraction pattern of the $60^\circ$ triangular lattice in the H-phase in Fig. 2(e), where peaks appear on a circle. The observation of this vortex lattice deformation may be another means to detect the fourfold-twofold transition in the $H$-$T$ phase diagram.

At higher field in the L-phase, we also find the vortex sheet structure in addition to the regular vortices. We show the spatial distribution of $|\eta_1(r)|$ and $|\eta_2(r)|$ at $H/H_c(0) = 0.3$ in Fig. 3(a). The black circle region presents regular vortex, where $|\eta_1(r)|$ and $|\eta_2(r)|$ share the same vortex core, as seen in Fig. 2(a). The green (red) circle region shows the $\eta_1$-$\eta_2$-vortex, where only $|\eta_1(r)|$ ($|\eta_2(r)|$) has vortex core and the other $|\eta_2(r)|$ ($|\eta_1(r)|$) does not. These green and red vortex cores are located alternatively along a loop, forming vortex sheet. In the internal field distribution shown in Fig. 3(b), $B(r)$ has a sharp localized peak at a regular vortex. And large $B(r)$ regions of the vortex core on the vortex sheet are connected each other along the vortex sheet. Each of $\eta_1$- and $\eta_2$-vortices has half flux quantum. If this line structure is found by the direct observation of the internal field distribution, it can be evidence of the vortex sheet appearing in unconventional superconductors. The relative phase of $\eta_1(r)$ and $\eta_2(r)$ are presented in Fig. 3(c). Around the regular vortex, the relative phase is fixed.
at \((\alpha + \pi)/2\) or \((\alpha - \pi)/2\) (in our parameter, \(\alpha = \pi\)).
Across the vortex sheet, the relative phase changes from 0 (red region) to \(\pi\) (blue region). This indicates that the vortex sheet appears at the domain wall between the region with the relative phase \((\alpha + \pi)/2\) and that with \((\alpha - \pi)/2\), and that it is not easy to disconnect vortices on the vortex sheet. As shown in the right panel in Fig. 4(c), since windings of the relative phase are opposite at the \(\eta_1\)-vortex and the \(\eta_2\)-vortex, the relative phase changes from 0 to \(\pi/2\) (yellow) or 3\(\pi/2\) (purple) alternatively between the nearest neighbor vortices along the vortex sheet. Since domains with relative phase \((\alpha \pm \pi)/2\) are degenerate in free energy, we can expect both domains to coexist in sample materials. In the presence of the domain wall between domains, vortex sheet appears when applying field. In our simulation for the penetration process of vortices, boundary region helps creation of the domain wall with vortex sheet structure. The domain wall and vortex sheet are tight structure when coming inside, and survive stably.

Lastly, we consider the case when the gradient coupling terms do not vanish. We show the results when \(C_{12x} = 0.2\) and \(C_{12y} = 0\) and the other parameters are kept same. We note that, if we consider the s+id-state (e.g. \(\phi_1(k) \propto 1 - (k_x^4 + k_y^4 + k_\lambda^4)\) and \(\phi_2(k) \propto k_x^2 - k_y^2\) \(\square\), \(C_{12y} = 0\). We see the similar vortex structure as in Figs. 2 and 3 in the L-phase. The field dependence of the order parameter maximum of \(|\eta_2(r)|\) is shown in Fig. 4. On raising field, \(|\eta_2|\) decreases, but it does not vanish at \(H^*\). \(|\eta_2|\) has finite value up to \(H_{c2}(T)\). Therefore, twofold symmetric order parameter \(\eta_2(r)\phi_2(k)\) is mixed in addition to the fourfold one \(\eta_1(r)\phi_1(k)\) in the H-phase \(\square\). That is, \(H^*\) is not a phase transition but the crossover field where \(\eta_2\) is enhanced in the vortex state. While the anomaly of the second order transition appears at \(T^*\) in the zero field case, the anomaly of the phase transition is not observed around \(H^*\) at finite fields.

In summary, we investigate the vortex state based on the two-component GL theory in the situation when the fourfold-twofold symmetric superconducting transition occurs. We estimate the transition field \(H^*\) where second order parameter \(\eta_2\) appears. However, \(H^*\) is changed to a crossover field when the gradient coupling terms exist, because the small \(\eta_2\) survives up to \(H_{c2}(T)\). In the L-phase below \(H^*\), the vortex lattice deforms from 60° triangular lattice due to the effect of the twofold-symmetric second order parameter. In the two-component superconductor, there is a possibility to observe the exotic vortex structure such as vortex sheet at the domain wall, where two order parameters have different vortex cores and these cores are alternatively located along a line. These characters of the vortex structure may be clear evidence of the fourfold-twofold symmetric double transition and unconventional multi-component superconductivity, if they are experimentally observed.

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