Instability of square vortex lattice in \( d \)-wave superconductors is due to paramagnetic depairing

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Effects of the paramagnetic depairing on structural transitions between vortex lattices of a quasi two dimensional \( d \)-wave superconductor are examined. It is found that, in systems with Maki parameter \( \alpha_M \) of order unity, a square lattice induced by a \( d \)-wave pairing is destabilized with increasing fields, and that a reentrant rhombic lattice occurs in higher fields. Further, a weak Fermi surface anisotropy competitive with the pairing symmetry induces another structural transition near \( H_{c2} \). These results are consistent with the structure changes of the vortex lattice in CeCoIn\(_5\) in \( H \parallel c \) determined from recent neutron scattering data.

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Recently, various novel superconducting (SC) properties have been found in the heavy fermion superconductor CeCoIn\(_5\) in magnetic fields. Among them, the discontinuous \( H_{c2} \)-transition \(^1\) and a new high field phase, identified with a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) vortex state \(^2\), have been the subjects of central interest in the research field. Quite recently, much attention has been paid, in turn, to the vortex lattice structure \(^3, 4, 5\), have been the subjects of central interest in this work, spatial variations parallel to \( H \) and magnitude of \( H \) will be taken into account. The contribution to the sign of Cooper pairs and the reciprocal lattice vectors of \( \Delta \) will be explained later. The normalized energy density \( \mathcal{F} \), where \( \varphi_\sigma(\mathbf{r}) = S^{-1/2} \sum_\mathbf{p} \varphi_\sigma(\mathbf{p}) e^{i \mathbf{p} \cdot \mathbf{r}} \), is the system area, and \( B_\sigma(\mathbf{k}) = \sum_\mathbf{p} \Delta_\mathbf{p}(-\mathbf{p}) - \mathbf{p} \cdot \mathbf{c}_\sigma \mathbf{p}_+ \), where \( \mathbf{p}_\pm = \mathbf{p} \pm \mathbf{k}/2 \). Effects of including a FS anisotropy will be explained later. The normalized pairing function \( \Delta_\mathbf{p} \) will be assumed hereafter to be \( \sqrt{2} \cos(2\phi_\mathbf{p}) \), where \( \phi_\mathbf{p} = \arctan(p_y/p_x) \). In \( H \parallel c \) of interest in this work, spatial variations parallel to \( H \) are, in the mean field theory, negligible in the equilibrium states in lower fields than the FFLO region \(^3\), just below \( H_{c2} \). For this reason, we can focus hereafter on the 2D model (1) to discuss CeCoIn\(_5\).

In deriving \( \mathcal{F} \) in \( H \parallel c \) from the model (1), two mixings neglected in Ref.\(^4\) need to be incorporated here: First, in expressing the SC order parameter \( \Delta \) in terms of the pairing symmetry of CeCoIn\(_5\) will also be discussed.

The theoretical method we use here is a straightforward extension of that in Ref.\(^4\) starting from the 2D BCS hamiltonian with a circular FS

\[
\mathcal{H} = \frac{d}{2} \sum_{\sigma=\pm} \int d^2 r \left( \varphi_\sigma(\mathbf{r}) \right)^\dagger \left[ \frac{(-i \nabla + eA)^2}{2m} - \sigma \mu H \right] \varphi_\sigma(\mathbf{r}) - \frac{|g|}{2} \int \frac{d^2 k}{(2\pi)^2} B^\dagger_\sigma(\mathbf{k}) B_\sigma(\mathbf{k}),
\]

de to arrive at an appropriate Ginzburg-Landau (GL) free energy density \( \mathcal{F} \), where \( \varphi_\sigma(\mathbf{r}) = S^{-1/2} \sum_\mathbf{p} \varphi_\sigma(\mathbf{p}) e^{i \mathbf{p} \cdot \mathbf{r}} \), \( S \) is the system area, and \( B_\sigma(\mathbf{k}) = \sum_\mathbf{p} \Delta_\mathbf{p}(-\mathbf{p}) - \mathbf{p} \cdot \mathbf{c}_\sigma \mathbf{p}_+ \), where \( \mathbf{p}_\pm = \mathbf{p} \pm \mathbf{k}/2 \). Effects of including a FS anisotropy will be explained later. The normalized pairing function \( \Delta_\mathbf{p} \) will be assumed hereafter to be \( \sqrt{2} \cos(2\phi_\mathbf{p}) \), where \( \phi_\mathbf{p} = \arctan(p_y/p_x) \). In \( H \parallel c \) of interest in this work, spatial variations parallel to \( H \) are, in the mean field theory, negligible in the equilibrium states in lower fields than the FFLO region \(^3\), just below \( H_{c2} \). For this reason, we can focus hereafter on the 2D model (1) to discuss CeCoIn\(_5\).

Below, we study changes of the vortex lattice structure induced by the Pauli paramagnetic depairing in a superconductor with a \( d \)-wave pairing. In the orbital limit with vanishing Maki parameter \( \alpha_M = \sqrt{2} H_{\text{orb}}(0)/H_{P}(0) \), the familiar enhancement of square lattice symmetry in higher magnetic fields and upon cooling is obtained, where \( H_{\text{orb}}(0) \) is the orbital limiting field in 2D case, and \( H_{P}(0) \) is the Pauli-limiting field. By contrast, our calculation using a Maki parameter \( \alpha_M > 2.5 \) shows a phase diagram similar to the observed one in CeCoIn\(_5\) \(^5\), where a reentry of the rhombic lattice region occurs with increasing \( H \), and suggests that effects of the pairing symmetry on the structure and orientation of the vortex lattice are weakened with increasing field by the paramagnetic depairing. In fact, a FS anisotropy competitive with the \( d \)-wave symmetry is found to, in higher fields, can change the orientation of the vortex lattice discontinuously. The present results strongly suggest that the main origin of the square to rhombic reentrant structural transition (ST) curve seen in CeCoIn\(_5\) is the paramagnetic depairing. In relation to this, the issue of the pairing symmetry of CeCoIn\(_5\) will also be discussed.
FIG. 1: One half of a unit cell of a vortex lattice in real space oriented (a) by the $d_{x^2-y^2}$-pairing function $\Delta_p$ or (b) by a four-fold FS anisotropy competitive with $\Delta_p$. A rhombic to square ST is driven by the squashing indicated by each solid arrow.

the global phase diagram was studied. However, it plays essential roles, together with the higher LL corrections, in studying stable lattice structures.

Then, $\Delta$ is expressed as $\Delta(\mathbf{r}) = a_0 \varphi_0(x,y) + a_4 \varphi_4(x,y)$ satisfying $\langle |\Delta|^2 \rangle_x = 1$, where, in the Landau gauge $\mathbf{A} = H x \hat{y}$, $\varphi_0 = (n!)^{-1/2}(r_H^{1/2}\partial \hat{\varphi}/\partial H)|\varphi_0(x,y)$, $\varphi_0(x,y) = C_0 \sum_n \exp[i(n y/r_H) + \pi n^2/2] - (k_n + x/r_H)^2/2)$ is the Abrikosov lattice solution in the $n = 0$ LL with the orientation of Fig.1(a), $r_H^{-1} = \sqrt{2H}$, and $\langle \quad \rangle_x$ denotes spatial average. The order parameter of the square to rhombic ST is $k^2 - \pi$, where $k(>0)$ is defined by $k^2 = \pi \cot(\gamma/2)$ in terms of the apex angle $\gamma$ (see Fig.1(a)).

The quadratic GL term $F_2$ takes the form

$$F_2 = N(0)[M_{00}a_0^2 + M_{44}[a_4^2 + M_{04}(a_0^*a_4 + a_4^*a_0)],$$

where

$$M_{n_1n_2} = \frac{1}{N(0)|g|} \delta_{n_1n_2} - \int_0^\infty d\rho_0 f(\rho_0) \times \int_{-\pi}^{\pi} \frac{d\phi_0}{2\pi} |\Delta_p|^2 L_{n_1n_2}(\rho_0) \exp(-|\rho_0|^2/2),$$

$$L_n(\mu) = L_n(|\mu|^2)$$

is the $n$th order Laguerre polynomial, $L_{44}(\mu) = \mu^4/\sqrt{24}$, $\mu_j = \rho_j(v_x - i v_y)/\sqrt{2r_H}$,

$$f(\rho) = 2\pi T \exp\left(-2\pi T \rho \frac{\xi_0}{l} \frac{\cos(2\mu B H \rho)}{\sinh(2\pi T \rho)}\right).$$

$l/\xi_0$ is a mean free path in the normal state normalized by the coherence length $l$, and $T_0$ is the (mean field) SC transition temperature in the case with $H = 0$ and $l = \infty$. Further, any spatial variation of the flux density was neglected. After diagonalizing eq.(2), the $H_{\phi}(T)$-curve is given by $M_{00}M_{44} - (M_{04})^2 = 0$. The eigenmode determining $H_{\phi}(T)$ takes the form $\Delta = \cos \varphi_0 + \sin \varphi_4$, where $\chi > 0$, and $\cos^2 \chi = (M_{44} - M_{00})/(M_{44} - M_{00})^2 + 4M_{04}^2$.

Next, let us turn to the analysis of the quartic GL term $F_4$, or equivalently, the Abrikosov factor $\beta_4$ determining the lattice structure. Hereafter, we use the gauge $\mathbf{A} = H x \hat{y}$. To express $F_4$ in a convenient form for numerical analysis, we use the relation

$$\Delta^{(n)}(r; \mu) = \exp(i\nu \cdot (-i\nabla + 2e\mathbf{A}))\varphi_n(x,y)$$

$$= \frac{\exp(-|\mu|^2/2)}{\sqrt{2\pi} \mu} \left(\mu^* - \frac{\partial}{\partial \mu}\right)^n [\exp(\mu^2/2) \times \varphi_0(x + \sqrt{2}r_H \mu, y)],$$

which can be obtained in the present gauge by extending the analysis in Ref.14 to the case with higher LLs. The function $\varphi_0(x, y)$ itself is given by taking the gauge, $\mu^* \to 0$ limit in eq.(5). Then, $F_4$ is expressed by

$$\frac{\mathcal{F}_4}{2N(0)} = \int_0^\infty d\rho_1 d\rho_2 d\rho_3 \left(\sum_{j=1}^3 \rho_j\right)^2 \mathcal{J}_4,$$

where

$$\mathcal{J}_4 = S^{-1} \int d^2r \int_{-\pi}^{\pi} \frac{d\phi_0}{2\pi} \text{Re} \left[ |\Delta_p|^4 \Delta(\mathbf{r}; -\mu_1) \Delta(\mathbf{r}; -\mu_2) \Delta(\mathbf{r}; -\mu_3) \right],$$

and

$$\Delta(\mathbf{r}; \mu_j) = \cos \chi \Delta^{(0)}(\mathbf{r}; \mu_j) + \sin \chi \Delta^{(4)}(\mathbf{r}; \mu_j).$$

Below, other higher order GL terms will not be considered. This assumption is not permitted if $\mathcal{F}_4 \leq 0$. We will neglect the narrow region close to $H_{\phi}(0)$ including the FFLO region [4,5] and focus on the field and temperature range with a positive $\mathcal{F}_4$. Then, by carrying out the $r$-integral and the $\mu_j$-derivatives in eq.(6), $\mathcal{J}_4$ is given by

$$\mathcal{J}_4 = \frac{k \cos^4 \chi}{\sqrt{2\pi}} \sum_{m,n} (-1)^{m+n} \int_{-\pi}^{\pi} \frac{d\phi_0}{2\pi} |\Delta_p|^4 \exp\left(-k^2(m^2 + n^2)/2\right)$$

$$- \frac{1}{2} \sum_{j=1}^3 |\mu_j|^2 \text{Re} \left[ e^{-\nu_0(1 + p_1 \tan \chi + p_2 \tan^2 \chi)}\right],$$

up to $O(\tan^2 \chi)$, where

$$p_0 = \frac{1}{2} (\mu_2^2 + (\mu_3^2)^2) - \frac{1}{4} (\mu_2 - \mu_3 - \mu_2^2)^2 = \frac{k}{\sqrt{2}} \left(n(\mu_2 + \mu_3 - \mu_2^2) + m(\mu_2 - \mu_3 - \mu_2^2)\right),$$

$$p_1 = \frac{1}{\sqrt{4}!} \left(\sum_{j=1}^4 \left(\frac{3}{4} - 3K_j^2 + K_j^4\right)\right),$$

$$p_2 = \frac{1}{\sqrt{4}!} \left(\sum_{j=1}^4 \left(\frac{3}{4} - 3K_j^2 + K_j^4\right)\right) + \left(\frac{3}{4} - 3K_j^2 + K_j^4\right),$$

$$K_j = \frac{9}{2} (1 - K_j^2)(1 - 2K_j^2),$$

$$K_j = \frac{1}{2} (\mu_2 + \mu_3 - \mu_2^2) - \frac{k(m + n)}{\sqrt{2}},$$

$$K_4 = \frac{1}{2} (\mu_2 + \mu_3 - \mu_2^2) + \frac{k(m + n)}{\sqrt{2}}.$$
and
\[ K_{2j-1} = \mu_{2j-1} + \frac{1}{2} \mu_2 + (-1)^j [\mu_3^* - \mu_1^* + \sqrt{2}k(m-n)] \]  
\( (j = 1, 2) \). As is shown in Fig.2, even the contribution of the O(\( \tan^2 \chi \)) term is quantitatively negligible, and, for this reason, higher order terms in \( \tan \chi \) were neglected above. The mixing or coupling, occurring through the \( k \)-dependent terms in \( p_0 \) and \( K_2 \), between the momenta \( \mathbf{p} \) on FS appearing in the gap function \( \Delta_p \) and the reciprocal lattice vectors leads to structural changes of the vortex lattice at a fixed orientation. By determining the \( k \)-value minimizing \( F_4 (> 0) \) at each \((H, T)\), structural changes of the vortex lattice have been examined.

As examples of calculation results following from eq.(9), we focus below on those for \( \alpha_M = 0 \) and 2.8. The resulting square to rhombic ST lines for these \( \alpha_M \) values are expressed in Fig.2 by thick solid curves under a fixed \( l/\xi_0 \), where \( t = T/T_{c0} \), and \( h = H/H_{orb}(0) \).

In our calculation, the square to rhombic ST illustrated in Fig.1(a) was of second order everywhere. In higher \( H \) where the paramagnetic depairing is more important, \( \alpha_M \)-dependence of the ST curve is striking: In the orbital limit where \( \alpha_M = 0 \), the square lattice becomes more rigid in higher \( H \), while it is limited, as in Fig.2, in the intermediate field range surrounded by a closed ST curve if \( \alpha_M > 2.5 \). This reentry of the rhombic lattice implies that the interplay between the orbital-depairing and the \( d \)-wave pairing symmetry, enhancing the square lattice and fixing the orientation of the vortex lattice, is weakened by the paramagnetic depairing. On the other hand, although the ST curve in low fields \( h \ll 1 \), where the paramagnetic depairing is ineffective, shows the expected behavior insensitive to \( \alpha_M \)-values, it is not quantitatively reliable because our approach assuming dominant roles of the lowest LL is valid in higher fields. In fact, the square lattice region seems to have been overestimated near the low \( T \) and low \( H \) corner.

Figure 2 implies that a reentrant and closed ST curve similar to that found from neutron scattering data of CeCoIn\(_5\) in \( H \parallel c \) follows from \( \alpha_M \) of order unity. Judging from such a large effect of a finite \( \alpha_M \), the paramagnetic depairing is expected to be the main origin of the reentrant ST curve in CeCoIn\(_5\). For comparison, an \( \alpha_M = 0 \) ST curve with effects of elastic thermal fluctuation \([11, 12]\) included is expressed in Fig.2 by open circles. The fluctuation is incorporated in the squashing elastic modulus following from eq.(9) via replacement
\[ k^2 \rightarrow k^2(1 - 3k^2\overline{w}^2/(4\pi^2)) \]  
\([12]\), where \( \overline{w}^2 \) is the mean square average of vortex displacement calculated in terms of the material parameters of CeCoIn\(_5\). The obtained result clearly shows that the fluctuation-induced mechanism is a minor contribution to the reentry of the rhombic lattice in CeCoIn\(_5\). Hereafter, two additional features seen in the experimental phase diagram will be discussed. First, the high \( H \) branch of the ST curve in Ref.\([6]\) has shown a negative slope even at lower \( T \) in contrast to the positive slope in Fig.2. Since the paramagnetic effect suppressing the square lattice is more effective at lower \( T \), the positive slope in the present calculation is reasonable. A possible origin changing the slope sign of the high \( H \) branch is the quasiparticle damping \( \xi_0/l \) due to the non-SC critical fluctuation. In Fig.3, we show \( l/\xi_0 \) dependence of the phase diagram in \( \alpha_M = 2.8 \) case. In the context of CeCoIn\(_5\), the quasiparticle mean free path

**Figure 2:** Square to rhombic ST (thick solid) curves and the corresponding \( H_{c2}(T) \) (thin solid curves) in the \( h-t \) phase diagram in the case with the Maki parameter 0 and 2.8, the circular FS, and the fixed value \( l = 20\xi_0 \). Each thick solid curve was obtained by neglecting the O(\( \tan^2 \chi \)) term in eq.(9). For \( \alpha_M = 0 \), the square lattice is realized everywhere above the ST curve, while it is limited for \( \alpha_M = 2.8 \) in the area surrounded by the open circles in the case with the Maki parameter 0 and 2.8. In higher \( M \), the paramagnetic depairing is effective, shows the expected behavior insensitive to \( \alpha_M \)-values.

**Figure 3:** ST lines and the corresponding \( H_{c2}(T) \) lines for the fixed value \( \alpha_M = 2.8 \) obtained for \( l = \infty \) (open circles and the upper dashed curve) and \( l = 14.5\xi_0 \) (thick and thin solid curves). When \( l = \infty \), the discontinuous \( H_{c2} \)-transition due to the paramagnetic depairing occurs in \( t \leq 0.13 \), and the Pauli-limiting field \( H_P \) corresponds to the value \( h = 0.505 \). Between the first order ST curve (lower dashed line) and \( H_{c2}(T) \) in \( \alpha_M = 2.8 \), the vortex lattice has the orientation indicated in Fig.1(b) \([6]\).
the square lattice and a rhombic one with $l$ is not due to impurity scatterings but rather should be a consequence of non-SC critical fluctuations. It has been argued [5] that this damping effect is not negligible in the high $H$ region close to $H_{c2}(0)$ of CeCoIn$_5$ in $H \parallel c$. As Fig.3 shows, effects of a nonvanishing $\xi_0/l$ on the high $H$ ST curve are quantitatively weak in agreement with our view that a large $\alpha_M$ is the main origin of the reentrant ST curve. Nevertheless, the high $H$ ST curve tends to approach a flat curve with decreasing $l/\xi_0$. In the low $T$ region dominated by the paramagnetic depairing, a quasiparticle damping suppressing the paramagnetic effect is more effective and slightly shifts the high $H$ branch upwardly, while it shifts this branch downwardly at higher $T$ where the orbital depairing is rather important. We expect an inclusion of a (unknown) $T$-dependence of $l$ to resolve this issue more satisfactorily.

The experimental phase diagram [6] also includes first order STs between the two orientations indicated in Fig.1(a) and (b) both above and below the field region of the square lattice. To understand this, we have also examined effects of a weak four-fold anisotropy of FS competitive, in orientation, with that of $\hat{\Delta}_p$ on the high $h$ region of the $\alpha_M = 2.8$ phase diagram by introducing the anisotropy, as in Ref. [10], through the replacement $|\hat{\Delta}_p|\rightarrow v_F(1-\beta \cos 4\phi_p)/\sqrt{1-\beta^2}$ ($\beta > 0$), and the density of states. When this $v_F$-anisotropy is more dominant, the vortex lattice begins to change with the fixed orientation of Fig.1(b). We find that, for a weak FS anisotropy with $\beta = 0.05$, a first order ST between the two orientations indicated in Fig.1 appears on the lower dashed curve in Fig.3, above which the square lattice and a rhombic one with $\gamma = 74.5$ degrees are nearly degenerate in energy with the orientation of Fig.1 (b). This result fixes our view on the high field side of the experimental phase diagram of CeCoIn$_5$ [6] and supports the picture that the closed and reentrant ST curve is due not to a FS anisotropy but to the $d_{z^2}$-wave-pairing symmetry of CeCoIn$_5$. Actually, if the in-plane FS anisotropy relevant to the superconductivity of CeCoIn$_5$ is characterized as a single four-fold anisotropy, it is quite unreasonable to ascribe both of the reentrant ST curve and the first order STs to such a single FS anisotropy. Further, bearing the result in Ref. [10] in mind, the fact that another first order ST in lower fields, where the finite $\alpha_M$ does not work, is limited to a narrow range ($< 0.5$ (T)) [6] is consistent with the weak FS anisotropy assumed here. We note that the states with the orientation of Fig.1(b) are limited to the range $h < 0.4$ irrespective of the $l/\xi_0$ value and, when $l = \infty$, are not realized near $H_{c2}(T)$ in contrast to the observation [6]. This supports the argument [5] that the quasiparticle damping is not negligible in understanding the region near $H_{c2}$ of CeCoIn$_5$.

In conclusion, the paramagnetic depairing easily destroys the square vortex lattice stabilized by a $d$-wave pairing and is believed to be the main origin of the reentrant square to rhombic structural transition curve found in CeCoIn$_5$ [6]. The present results indicate that the paramagnetic depairing plays unexpectedly crucial roles in the high $H$ vortex lattice structure and may be the main origin of other field-induced lattice structure transitions such as the square to rhombic one in TmNi$_2$B$_2$C with a four-fold anisotropic Fermi surface [13].

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