The Effects of $d_{x^2-y^2}-d_{xy}$ Mixing on Vortex Structures and Magnetization

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Abstract

The structure of an isolated single vortex and the vortex lattice, and the magnetization in a $d$-wave superconductor are investigated within a phenomenological Ginzburg-Landau (GL) model including the mixture of the $d_{x^2-y^2}$-wave and $d_{xy}$-wave symmetry. The isolated single vortex structure in a weak magnetic field is studied both numerically and asymptotically. Near the upper critical field $H_{c2}$, the vortex lattice structure and the magnetization are calculated analytically.

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I. INTRODUCTION

Since the discovery of the high temperature superconductors (HTSC’s), a great number of experimental and theoretical investigations have been carried out to identify the symmetry of the superconducting pairing state. Although there still remain controversies, it is believed that the $d_{x^2-y^2}$-wave symmetry is most probable in HTSC’s; e.g. a series of strong evidences have been provided by the phase sensitive experiments.

In recent years, the structure of vortices in a $d_{x^2-y^2}$ superconductor was of great interest. It was expected that the structure of $d$-wave vortices might be very different from that of $s$-wave vortices. And connected with the vortex structure, the question of order parameter symmetry admixture arose.

From a standpoint of the spontaneous symmetry breaking, in a bulk with a perfect crystal symmetry, the order parameter transforms according to an irreducible representation of the crystallographic point group. Thus in a crystal of tetragonal ($D_4$) symmetry, only one symmetry state (e.g. $d_{x^2-y^2}$-wave) is allowed. However near interfaces, surfaces or impurities, the crystalline symmetry is not perfect and the $d_{x^2-y^2}$-wave order parameter fluctuates spatially and hence induces components of other symmetry. This is also the case in the presence of vortices, to which we will confine ourselves in this work.

Soininen et al., starting from a simple microscopic model Hamiltonian and its Bogoliubov-de Gennes equation, found a substantial admixture of an induced $s$-wave and the dominant $d_{x^2-y^2}$-wave. Based on this work, Berlinsky et al. and Franz et al. investigated the structure of $d$-wave vortices using the Ginzburg-Landau(GL) theory. Ren et al. microscopically derived the GL equation from the Gorkov equation of a continuum mean field model, and it was studied in detail by Xu et al. for the $d$-wave vortex structures. Joynt also included the $d$-$s$ mixing term in their phenomenological GL model, from the symmetry argument. Very recently, Maki and Béal-Monod and Won and Maki also incorporated $d$-$s$ mixture. They used an interaction potential with the $s$ channel repulsive Coulomb interaction in their weak-coupling model. In most of the works above, they ob-
served that the $s$-wave component induced near the vortex core causes the $d$-wave component to have fourfold anisotropy and that the vortices arrange in an oblique lattice instead of triangular one.

Recently, the possibility of admixture of $d_{x^2-y^2}$-wave and $d_{xy}$-wave was also suggested. Koyama and Tachiki took into account the internal orbital motion of the pairing electrons in their linearized Gorkov-type gap equation near $T_c$. They found that the dominant $d_{x^2-y^2}$-wave symmetry was mixed with $d_{xy}$-wave symmetry, instead of the $s$-wave. The coupling of the two $d$-wave components led to a significant paramagnetic effect and to strong enhancement of the upper critical field at lower temperatures, which remarkably fits the experimental results on over-doped cuprate superconductors Bi$_2$Sr$_2$CuO$_y$ and Tl$_2$Ba$_2$CuO$_6$. And Ichioka et al. considered both $d_{x^2-y^2}$-$s$ mixing and $d_{x^2-y^2}$-$d_{xy}$ mixing in the framework of the classical Eilenberger equations. They studied the isolated single vortex structures and found that the amplitude of the $d_{xy}$-wave component has the shape of an octofoil.

As described above, for the case of $d$-$s$ mixture, the single vortex and/or vortex lattice structure have been extensively studied, but not for the case of $d_{x^2-y^2}$-$d_{xy}$ mixture. In this paper, we present analogous studies based on the GL theory which includes the mixing of $d_{x^2-y^2}$-wave and $d_{xy}$-wave, assuming the $d_{x^2-y^2}$-wave symmetry of the superconducting ground state.

II. GL THEORY FOR A $D$-WAVE SUPERCONDUCTOR

We start with the GL free energy functional proposed by Koyama and Tachiki:

$$G(H) = \int (dx) \left\{ \frac{\hbar^2}{4m_+} \left| \left( -i\nabla + \frac{2\pi}{\phi_o} \mathbf{A} \right) \Psi_+ \right|^2 + \alpha_+ (T) \left| \Psi_+ \right|^2 + \frac{1}{2} \beta_+ \left| \Psi_+ \right|^4 
+ \frac{\hbar^2}{4m_-} \left| \left( -i\nabla + \frac{2\pi}{\phi_o} \mathbf{A} \right) \Psi_- \right|^2 + \alpha_- \left| \Psi_- \right|^2 + \frac{1}{2} \beta_- \left| \Psi_- \right|^4 
+ \beta_X \left| \Psi_+ \right|^2 \left| \Psi_- \right|^2 + \beta_Y \left| (\Psi_+^* \Psi_-^2 + h.c.) \right| - \frac{1}{2} \gamma_p \left( \Psi_+^* \Psi_- + h.c. \right) B_z 
+ \frac{B^2}{8\pi} \frac{\mathbf{B} \cdot \mathbf{H}}{4\pi} \right\},$$

(1)
where the order parameter $\Psi_+ (\Psi_-)$ corresponds to the $d_{x^2-y^2}$-wave ($d_{xy}$-wave) symmetry. As we previously assumed, in Meissner state, the only non-vanishing component is $\psi_+$ and $\alpha_+(T) < 0$ at $T < T_c$. Other coefficients are assumed to be positive and independent of temperature.

In passing, we make a couple of remarks. In Eq. (1) we included the coupling term $\sim (\Psi_+^2\Psi_-^2 + h.c.)$, which was omitted in the model originally proposed by Koyama and Tachiki. This term is necessary in order to get the most general (up to the fourth order) free energy functional from the symmetry consideration. The mixing term $\sim (\Psi_+^*\Psi_- + h.c.)B_z$ in the quadratic order give rise to the paramagnetic current. As we will see below, it dominates other mixing terms and significantly affects the mixed state properties of $d$-wave superconductors.

In mean field approximation, neglecting thermal fluctuation effects, physical properties are described by the corresponding GL equations. It is convenient to introduce the dimensionless quantities by adopting the fundamental length scale to be the GL coherence length $\xi_+$ of $\Psi_+$ (See Table. I). In this case, the GL equations and Maxwell equations are written as

$$\Pi^2\psi_+ - \psi_+ + |\psi_+|^2\psi_+ + \chi_+|\psi_-|^2\psi_+ + \zeta_+\psi_+^*\psi_-^2 - \nu_+ B_z\psi_+ = 0,$$

(2)

$$\Pi^2\psi_- + \Xi\psi_- + \Upsilon|\psi_-|^2\psi_- + \chi_-|\psi_+|^2\psi_- + \zeta_-\psi_-^*\psi_+^2 - \nu_- B_z\psi_- = 0,$$

(3)

$$\kappa^2\mathbf{J} = -\frac{1}{2}(\psi_+^*\Pi\psi_+ + h.c.) - \frac{1}{2}\mu^{-1}(\psi_-^*\Pi\psi_- + h.c.)$$

$$+ \frac{1}{2}\nu_+ \nabla \times (\psi_+^*\psi_- + h.c.)\hat{z},$$

(4)

where $\nabla \times \nabla \times \mathbf{A} = \mathbf{J}$ and $\Pi = (-i\nabla + \mathbf{A})$ and other parameters are defined in the Table I. In Eq. (I), the last term is the paramagnetic current contribution.

### III. ISOLATED SINGLE VORTEX STRUCTURE

Consider an isolated single vortex near the lower critical field $H_{c1}$. For the problem of isolated single vortex, it would be convenient to decompose the order parameter into the
form \( \psi_\pm = f_\pm e^{i\varphi_\pm} \). Since the \( d_{xy} \)-wave component is induced through the direct coupling to the magnetic field, in the low field near \( H_{c1} \) its amplitude is expected to be very small compared with \( d_{x^2-y^2} \)-wave component. Thus just for intuitive understanding, for a moment we neglect the effect of the coupling in the fourth order (\( \chi_\pm = 0, \zeta_\pm = 0 \)). The effect will be considered below.

Let’s first look at the phase distributions associated with the vortex. It is obvious from the rotational symmetry of the GL equations that the phases should have \( \varphi(r, \theta)_\pm = -\theta \) up to an additive constant, which we take to be zero; the two \( d \)-wave components have the same winding. Thus, the differential equations are rewritten, in terms of \( f_\pm \) only, as

\[
\Pi^2 f_+ - f_+ + f_+^3 - \nu_+ B f_- = 0 
\]

\[
\Pi^2 f_- + \Xi f_- + \Upsilon f_-^3 - \nu_- B f_+ = 0 
\]

\[
\kappa^2 J = -(f_+^2 + \mu^{-1} f_-^2) (-1/r + A)\hat{\theta} + \nu_+ \nabla \times (f_+ f_-)\hat{z}, 
\]

where \( \Pi^2 = -\frac{d^2}{dr^2} - \frac{1}{r} \frac{d}{dr} + \left( -\frac{1}{r} + A \right)^2 \), \( A = A(r)\hat{\theta}, \ B = B(r)\hat{z} \), and \( J = J(r)\hat{\theta} \).

Second, near the vortex center \( r \to 0 \), \( B(r) \) and \( f_\pm(r) \) have the asymptotic behavior of the following form:

\[
B(r) = B_0 + B_2 r^2 + O[r^4] 
\]

\[
f_+(r) = C_0 r \left(1 + C_2 r^2 + O[r^4]\right) 
\]

\[
f_-(r) = D_0 r \left(1 + O[r^4]\right) 
\]

where\[\]

\[
C_2 = -\frac{1}{8} (1 + B_0) \left[ 1 + \nu^2 \frac{B_0^2}{\Xi - B_0}(1 + B_0) \right] 
\]

\[
D_0 = \nu_2 \frac{B_0}{\Xi - B_0} C_0 
\]

\[
B_2 = -\frac{1}{2} \frac{C_0^2}{\kappa^2} \left[ 1 - 2\nu^2 \frac{B_0}{\Xi - B_0} + \nu^2 \left( \frac{B_0}{\Xi - B_0} \right)^2 \right] 
\]
Note that since $B_0 \sim 2/\kappa^2$, in the extreme type-II superconductors ($\kappa \gg 1$) the asymptotic behaviors of $B(r)$ and $f_+(r)$ deviates very little from those of the conventional $s$-wave GL theory ($C_2 \simeq -(1 + B_0)/8$, $B_2 \simeq -C_0^2/2\kappa^2$).

Next, consider the region far from the vortex center ($r \gg \kappa$). Assuming the extreme type-II superconductor ($\kappa \gg 1$), we can treat $f_+ = 1$ and neglect $|\nabla^2 f|_+ \sim f_-/\kappa^2 \ll f_-$. Then by taking the curl of Eq. (7) we get the usual London equation:

$$\kappa^2 \nabla \times \nabla \times B + B = 2\pi \delta^2(r),$$

and from Eq. (13)

$$f_+(r) \simeq \frac{\nu}{\Xi} B(r) \sim \sqrt{\kappa/r} e^{-r/\kappa}, \quad (r \gg \kappa).$$

Thus far outside the core, only the pure $d_{x^2-y^2}$-wave component remains.

Now we discuss the effect of the mixing terms in the fourth order, i.e. with finite $\chi_\pm$ and $\zeta_\pm$. In general, due to the coupling of the form $(\psi_+^2 \psi_-^2 + h.c.)$ the GL equations do not have spherical symmetry. However, within the assumption of small $d_{xy}$-wave component, we can apply a partial wave expansion for $\psi_-:

$$\psi_- = \sum_n f_-^{(n)}(r)e^{in\theta}.$$ 

It is straightforward to show that the only non-vanishing component is of $n = 1$, and that the asymptotic results given above have no change.

We also provide the numerical results for the distribution of the order parameter and the magnetic induction in Fig. 1. As shown in the Fig. 1 (a), the magnitude $f_-(r)$ of the $d_{xy}$-wave component increases as the $d_{x^2-y^2}$-$d_{xy}$ coupling strength $\nu_+$ ($\nu_-$) increases and as the temperature $T$ decreases. However, $f_-(r)$ is so small that its effect on $f_+(r)$ and $B(r)$ is negligible; the isolated single vortex structure of this model is very similar to that of the conventional $s$-wave GL theory.
IV. VORTEX LATTICE AND MAGNETIZATION NEAR THE UPPER CRITICAL FIELD

In the vicinity of the upper critical field $H_c^2$, the magnitudes of the order parameters are small and thus the non-linear terms in the GL equations Eqs. (2,3) are negligible. The magnetic field are also assumed to be constant all over the space since the inter-vortex spacing is much less than the penetration depth $\lambda_+$. Then the GL equations are reduced to a linearized form:

\begin{align}
(\Pi^2 - 1)\psi_+ - \nu_+ B_z \psi_&= 0, \quad (17) \\
(\Pi^2 + \Xi)\psi_- - \nu_- B_z \psi_&= 0. \quad (18)
\end{align}

Each of the solutions $\psi_{L\pm}$ is just a linear combination of the wave functions in the lowest Landau level, which is infinitely degenerate, and determined so as to minimize the GL free energy.

We minimize the free energy by generalizing the Abrikosov’s procedures. In these procedures, the two components of the order parameter satisfy

\begin{equation}
\frac{\psi_{L-}}{\psi_{L+}} = \frac{1}{\nu_+} \frac{H_{c2} - 1}{H_c^2}, \quad (19)
\end{equation}

and that the current contribution is given by

\begin{equation}
\kappa^2 J_L = -\frac{1}{2} \nabla \times \left\{ |\psi_{L+}|^2 + \mu^{-1} |\psi_{L-}|^2 - \nu_+ (\psi^*_{L+} \psi_{L-} + h.c.) \right\} \hat{z}. \quad (20)
\end{equation}

Then the magnetization and the GL free energy are given by

\begin{equation}
4\pi M = -\frac{H_{c2} - H}{(2\kappa^2_{\text{eff}} - 1)\beta_A}, \quad (21)
\end{equation}

\begin{equation}
G_s(H) = G_n(H_{c2}) + 2\kappa^2 \left[ (H_{c2}^2 - H^2) - \frac{(H_{c2} - H)^2}{(2\kappa^2_{\text{eff}} - 1)\beta_A} \right] \quad (22)
\end{equation}

where $\beta_A \equiv \langle f^4 \rangle / \langle f^2 \rangle^2$ is a still undetermined parameter, and $\kappa^2_{\text{eff}}(T) = \kappa^2 G(T) / F^2(T)$ with
\[
R(T) = \frac{1}{\nu_+} \frac{H_{c2}(T) - 1}{H_{c2}(T)} \\
F(T) = 1 - 2\nu_+ R + \mu^{-1} R^2 \\
G(T) = 1 + 2(\chi_+ + \zeta_+) R^2 + \mu^{-1} \Upsilon R^4.
\]

The Abrikosov parameter \(\beta_A\) concerns the vortex lattice structure and is determined by minimizing the GL free energy. Since \(\psi_{L+}\) has the same form as the \(s\)-wave Abrikosov solution, it is obvious that the free energy is minimized for the triangular vortex lattice \((\beta_A = 1.16)\). The magnetization in Eq. (21) shows the usual form of the conventional \(s\)-wave GL theory\(^{22,23}\), but the slope \(4\pi dM/dH\) depends on the temperature.

V. DISCUSSIONS

There is no direct observation of the single vortex structure in a HTSC, while Keimer \etal\(^{26}\) and Maggio-Aprile \etal\(^{27}\) observed oblique lattices in their SANS and STM experiments on YBCO compound, respectively. Their result of oblique lattice is not consistent with our result of triangular lattice. Both the single vortex structure and the vortex lattice structure is also different from theoretical predictions based on the \(d_{x^2-y^2}\)-\(s\) admixture scenario\(^{7,8,10,11,14}\).

The single vortex structure can have a significant influence on the structure of the vortex lattice in many-vortex problem. It is quite interesting to note that the four-fold symmetry of \(d-s\) admixed vortex is an implication of the mixed gradient coupling in its model. In our model, there is no mixed gradient term up to quadratic order. Very recently, Ichioka \etal\(^{16}\) argued that a non-local correction is required and associated GL theory should enclose the fourth order mixed gradient term. They observed that the \(d_{x^2-y^2}\)-wave component has the four-lobe shape and \(d_{xy}\)-wave component the shape of octofoil. Although in this present paper we put emphasis on the effect of mixing through the direct coupling to the magnetic field, the result of Ichioka \etal. strongly suggests that the \(d_{x^2-y^2}-d_{xy}\) admixture can leads to an oblique vortex lattice. Furthermore, even in the present GL model, for the intermediate field regime off the extreme regions near to \(H_{c1}\) or \(H_{c2}\), the order parameter distribution is
not spherically symmetric. Therefore further study is required for that region, because the non-spherical symmetry of the supercurrent distribution around a vortex is not compatible with the triangular lattice symmetry.

The strong temperature dependence of $\kappa_{\text{eff}}(T)$ in Eq. (21) reminiscent of $\kappa_2(T)$ in the microscopic consideration of conventional superconductors by Maki and Eilenberger. Roughly speaking, the difference between $\kappa_2(T)$ and $\kappa$ for that case was due to the non-locality of the electromagnetic response of the superconductors. In our case, the strong $T$-dependence of $\kappa_{\text{eff}}(T)$ has an interesting interpretation. In contrast to the low field limit, $\psi_-$ is order of $\psi_+$ at high fields ($H \sim H_{c2}$) and low temperatures for $\nu_p \sim 1$, and the associated paramagnetic current significantly affects the magnetization curve $4\pi M(H)$ in low temperature region. Several experiments reported the strong temperature dependence of the slope $4\pi dM/dH$ near $H_{c2}(T)$ in HTSC.

VI. CONCLUSIONS

We investigated a GL theory for vortex structures and magnetization in a $d$-wave superconductor. In the GL theory, we assumed the $d_{x^2-y^2}$-wave symmetry of the superconducting ground state, and the admixture of $d_{x^2-y^2}$-wave and $d_{xy}$ symmetry in the presence of the vortices. The structure of an isolated single vortex was studied asymptotically and numerically at low field region ($H \sim H_{c1}$). The isolated single vortex is similar to conventional $s$-wave vortex, and has almost spherically symmetric supercurrent distribution around it. The vortex lattice structure and magnetization were studied analytically at high fields near the upper critical field $H_{c2}$. The vortices arrange in a triangular lattice, and the magnetization curve $4\pi M(H)$ shows a strong temperature dependence for $\nu_p \sim 1$ due to the paramagnetic current effect. Some physical implications of the results were discussed. The results were also compared with the experimental observations and with those of $d$-$s$ scenario. It was recognized that further study in the intermediate field region is valuable.
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17 In the work of Koyama and Tachiki, the GL free energy functional was derived only up to quadratic order.

18 It should be noted that the order parameters have been defined in an unconventional
way [See Koyama and Tachiki (1996)]. The time-reversal operation, which transforms
\( \Psi_+ \rightarrow \Psi_+^*, \, \Psi_- \rightarrow -\Psi_-^*, \) and \( B \rightarrow -B, \) leaves the mixing term invariant.

19 The inter-vortex distance is much larger than the penetration depth.

20 Precisely speaking, the necessary condition is \( \varphi(r, \theta) = n\theta + C \) (with \( n \) integer). But the lowest energy states correspond to \( n = \pm 1, \) and we take \(-1\) just for a convenience.

21 \( C_0 \) is related to \( B_0, \) and determined by going higher order.

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TABLES

TABLE I. Characteristic lengths, scales of physical quantities, and phenomenological parameters in the GL theory in question.

| Characteristic lengths  | $\xi_+^2 = \frac{\hbar^2}{4m_+|\alpha_+|}$, $\xi_-^2 = \frac{\hbar^2}{4m_-\alpha_-}$, $\lambda_+^2 = \frac{m_+c^2}{8\pi e^2|\Psi_o|^2}$ |
|------------------------|------------------------------------------------------------------------------------------------------------------|
| Characteristic field$^a$| $H_{o2}^c = \phi_0/2\pi\xi_+^2$                                                                                   |
| Fundamental parameters | $\Psi_o^2 = |\alpha_+|/\beta_+$, $\Phi_0/2\pi = \hbar c/2e$, $\kappa = \lambda_+ / \xi_+$                     |
| Auxiliary parameters   | $\Xi = \xi_+^2/\xi_-^2$, $\Upsilon = m_-\beta_-/m_+\beta_+$, $\mu = m_-/m_+$, $\nu_\pm = \gamma_\rho m_\pm e/\hbar$, $\nu_p^2 = \nu_+\nu_-$, $\chi_+ = \beta \chi/\beta$, $\chi_- = \mu \chi_+$, $\zeta_+ = \beta \zeta/\beta$, $\zeta_- = \mu \zeta_+$ |
| Reduced units          | $\Psi_\pm / \Psi_o = \psi_\pm$, $T/T_c \to T$, $r/\xi_+ \to r$, $B/H_{o2}^c \to B$, $A/\xi_+H_{o2}^c \to A$, $J/(cH_{o2}^c/4\pi \xi_+) \to J$ |

$^a$ Here $H_{o2}^c$ is not the true upper critical field. The upper critical field can be substantially enhanced in this model.
FIGURES

FIG. 1. Distribution of the magnitudes of the order parameter and the magnetic induction associated with an isolated single vortex, for different values of $T$ and $\nu_+': T = 0.1, 0.9$ and $\nu_+ = 0.1, 0.9$. Other parameters are set as $\mu = 1.0, \Xi(0) = 1.0, \Upsilon = 1.0, \chi_+ = 0.8$.

FIG. 2. Temperature dependence of the $\kappa^2_{\text{eff}}$ for three different values of $\nu_p$. Other parameters are set as $\mu = 1.0, \Xi(0) = 1.0, \Upsilon = 1.0, \chi_+ = 0.8$. 
