Superconducting state properties of a $d$-wave superconductor with mass anisotropy

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Abstract

YBa$_2$Cu$_3$O$_7$ (YBCO) exhibits a large anisotropy between the $a$ and $b$ axes in the CuO$_2$ planes because of the presence of CuO chains. In order to account for such an anisotropy we develop a Ginzburg-Landau (GL) theory for an anisotropic $d$-wave superconductor in an external magnetic field, based on an anisotropic effective mass approximation within CuO$_2$ planes. The anisotropic parameter $\lambda = m_x/m_y$, where $m_x$ ($m_y$) is the effective mass in the $x$ ($y$) direction, is found to have significant physical consequences: In the bulk case, there exist both the $s$- and $d$-wave order parameters with the same transition temperature, as long as $\lambda \neq 1$. The GL equations are also solved both analytically and numerically for the vortex state, and it is shown that both the $s$- and $d$-wave components show a two-fold symmetry, in contrast to the four-fold symmetry around the vortex, as expected for the purely $d$-wave vortex. With the deviation of $\lambda$ from unity, the opposite winding between the $s$- and $d$-wave components observed in the purely $d$-wave case is gradually taken over by the same winding number. The vortex lattice is found to have oblique structure in a wide temperature range with the precise shape depending on the anisotropy.

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I. INTRODUCTION

Recently, the order parameter symmetry has become the central issue in high-$T_c$ superconductivity. Many experiments which probe directly the phase of the pairing state have provided strong evidence for a sign change of the order parameter [1, 2], consistent with a predominantly $d$-wave pairing symmetry. At the same time, there are several measurements which cannot be explained within the simple $d_{x^2-y^2}$ state. For example, finite tunneling current along the $c$ axis of a copper oxide clearly shows an $s$-wave character [3], because there should be no Josephson current between a CuO$_2$ plane with a gap of $d_{x^2-y^2}$ symmetry and a conventional $s$-wave superconductor.

It is well known that YBCO is not in the purely tetragonal phase due to the existence of chains. Indeed, YBCO exhibits a large anisotropy between the $a$ and $b$ directions in the measurements of the penetration depth [4] and the vortex structure by scanning tunneling microscopy (STM) [5]. It was argued recently [6] that these apparently conflicting experimental results in this material may be explained by assuming that there exist two order parameters, with different symmetry but the same transition temperature. Namely, the main gap with a $d$-wave symmetry would result from the CuO$_2$ planes, and a smaller $s$-wave component would be due to the CuO chains.

In this work, we will consider a simple model for an anisotropic $d$-wave superconductor, based on the anisotropic effective mass approximation within a single CuO$_2$ plane. In this model, the $a$-$b$ anisotropy of YBCO is taken into account by a single parameter, namely the electron mass anisotropy, $\lambda = m_x/m_y$, which can be fit to the measured penetration depth anisotropy [3]. Then the Ginzburg-Landau (GL) theory for such an anisotropic $d$-wave superconductor will be studied. Following the procedure described in Ref. [9], we first derive microscopically the GL equations for this anisotropic system, and then consider the possible solutions of these GL equations for both bulk and vortex states. We will show that the anisotropic parameter $\lambda$ has significant physical consequences: in the bulk, the stable solution from our theory is the mixed $s+d$ state, and both the $s$- and $d$-wave order parameters have the same transition temperature. This $s+d$ state is just what we want to explain the tunneling data and other apparently conflicting results observed in YBCO. The GL equations are also solved both analytically and numerically for the vortex structures. We find that the anisotropic $d$-wave vortex is very different from the purely $d$-wave case. Namely, both the $s$- and $d$-wave components show a two-fold symmetry, in contrast to the four-fold symmetry around the vortex as expected for the purely $d$-wave vortex. Specifically, the $d$-wave order parameter exhibits an elliptic shape and the $s$-wave component shows a shape of butterfly. With the deviation of $\lambda$ from unity, the opposite winding between the $s$- and $d$-wave components obtained in the purely $d$-wave case [4] is gradually taken over by the same winding number. The vortex lattice is found to be in oblique in a wide temperature range with the precise shape depending on the anisotropic parameter $\lambda$. Here we wish to point out that the preliminary results of $\lambda = 1$ case for the structures of a single vortex and vortex lattice were reported recently in a conference on superconductivity [10]. Here we concentrate on the results for the $\lambda \neq 1$ case.

In Sec. II, starting from Gorkov’s theory of weakly coupled superconductors [11], the GL equations for the anisotropic $d$-wave superconductor are derived. In Sec.III, we discuss the possible solutions of the GL equations for a uniform or bulk system. In Sec.IV, we
study analytically the qualitative features of a single vortex using the GL equations. In Sec.V, we present the numerical result for single vortex structure. The numerical calculation for a vortex lattice structure is performed in Sec.VI, and Sec.VII includes conclusion and discussions.

II. GL EQUATIONS

In this section we shall derive the GL equations for the anisotropic $d$-wave superconductor, following closely the procedure we used for a purely $d$-wave superconductor. Here only the main steps are presented and the difference between the present work and the previous one will be emphasized. Our starting point is the gap equation

$$\Delta^*(x, x') = V(x - x')T \sum_{\omega_n} F^\dagger(x, x', \omega_n),$$

which allows for more general than conventional $s$-wave pairing. $V(x - x')$ is the effective two-body interaction of the weak-coupling theory. Using Gorkov description of a superconductor in the magnetic field:

$$\left[ i\omega_n - \frac{1}{2m}(-i\nabla + eA)^2 + \mu \right] \tilde{G}(x, x', \omega_n) + \int dx'' \Delta(x, x'') F^+(x'', x', \omega_n) = \delta(x - x'),$$

$$\left[ -i\omega_n - \frac{1}{2m}(i\nabla + eA)^2 + \mu \right] F^+(x, x', \omega_n) + \int dx'' \Delta^*(x, x'') \tilde{G}(x'', x', \omega_n) = 0,$$

where $\mu$ is the Fermi energy and $A$ is the vector potential. The normal-state Green’s function at zero magnetic field can be written in the form

$$G_0(x, \omega_n) = \frac{1}{(2\pi)^2} \int \frac{dk}{i\omega_n - \xi_k},$$

where

$$\xi_k = \frac{k_x^2}{2m_x} + \frac{k_y^2}{2m_y} - \mu,$$

is the single particle energy measured from the Fermi energy $\mu$. We note that the case with $m_x = m_y$ in the above equation corresponds to the isotropic $d$-wave superconductor. Keeping up to the third order in $\Delta$, defining the central-mass coordinates $R = (x + x')/2$ and the relative coordinates $r = x - x'$, and making Fourier transform with respect to the relative coordinates, we obtain

$$\Delta(R, k) = \int \frac{dk'}{(2\pi)^2} V(k' - k)T \sum_{\omega_n} \frac{1}{\omega_n^2 + \xi_k'^2} \Delta(R, k')$$

$$+ \int \frac{dk'}{2(2\pi)^2} V(k' - k)T \sum_{\omega_n} \left[ \frac{\xi_k'^2 - 3\omega_n^2}{\omega_n^2 + \xi_k'^2} \left( \frac{k_x'^2}{2m_x^2} + \frac{k_y'^2}{2m_y^2} \right) \right] \Delta(R, k')$$

$$- \int \frac{dk'}{(2\pi)^2} V(k' - k)T \sum_{\omega_n} \frac{1}{\omega_n^2 + \xi_k'^2} |\Delta(R, k')|^2 \Delta(R, k'),$$

(2.6)
where we have introduced the operator
\[ \Pi = i \nabla_R - 2e A_R. \] (2.7)

In order to obtain the generic Ginzburg-Landau equations, which govern the spatial variation of the order parameters, for an anisotropic \( d \)-wave superconductor, we need to specify the form of the interaction. Here we use the following ansatz for the effective interaction responsible for the spin-singlet pairing:
\[ V(k - k') = -V_s + V_d(\hat{k}_x^2 - \hat{k}_y^2)(\hat{k}_x'^2 - \hat{k}_y'^2), \] (2.8)
where \( \hat{k} = k/|k| \) is the unit vector in the direction of \( k \). By taking both \( V_d \) and \( V_s \) positive, the \( -V_d \) corresponds to attractive interaction responsible for \( d \)-wave pairing, and \( V_s \) can be regarded as an effective on-site repulsive interaction. The general expression of order parameter that follows Eq.(2.8) is
\[ \Delta(R, k) = \Delta_s(R) + \Delta_d(R)(\hat{k}_x^2 - \hat{k}_y^2). \] (2.9)

Substituting Eqs.(2.8) and (2.9) into Eq.(2.6), and Comparing both sides of the gap equation for \( \hat{k} \)-independent terms and terms proportional to \( (\hat{k}_x^2 - \hat{k}_y^2) \), we obtain the GL equations in a form suitable for finding the GL free energy functional:
\[ \alpha_s \Delta_s - \frac{\lambda - 1}{\lambda + 1} \Delta_d + 2 \alpha \gamma_d \mu \left\{ \left( \frac{\Pi_x^2}{2m_x} + \frac{\Pi_y^2}{2m_y} \right) \right\} \Delta_s \]
\[ + \left[ \frac{\lambda + 2 \sqrt{\lambda} - 1}{(1 + \sqrt{\lambda})^2} \frac{\Pi_x^2}{2m_x} - \frac{2 \sqrt{\lambda} + 1 - \lambda}{(1 + \sqrt{\lambda})^2} \frac{\Pi_y^2}{2m_y} \right] \Delta_d \]
\[ + 2 \gamma_d \alpha \left[ \Delta_s^2 \Delta^* + \frac{\sqrt{\lambda} - 1}{\sqrt{\lambda} + 1} |\Delta_s|^2 \Delta_d + \frac{\lambda + 1}{(1 + \sqrt{\lambda})^2} \Delta_s^* \Delta_d^* \Delta_d \right] + \frac{\lambda + 1}{(1 + \sqrt{\lambda})^2} \Delta_s^2 \Delta_d^2 = 0, \] (2.10)

where \( \alpha = 7 \zeta(3)/8(\pi T)^2 \), \( \gamma \) is the Euler constant, \( \gamma_d = N(0)V_d/2 \) is the interaction strength in the purely \( d \)-wave channel when \( \lambda = 1 \), and
It is easy to show that if setting $\lambda = 1$, Eqs.(2.10) and (2.11) return back to the results we obtained for a purely $d$-wave superconductor \[9\]. The corresponding GL free energy is

\[
F = \left[1 - \gamma_d \ln \left(\frac{2e^\gamma \omega_D}{\pi T}\right) + \frac{2(1+\lambda)}{(1+\sqrt{\lambda})^2} |\Delta_d|^2 + \alpha_s |\Delta_s|^2 - \frac{\lambda - 1}{\lambda + 1} (\Delta_s^* \Delta_d + \Delta_d^* \Delta_s)\right]
\]

\[
+ 2\gamma_d \alpha \mu \left[\frac{|\Pi_x \Delta_s|^2}{2m_x} + \frac{|\Pi_y \Delta_s|^2}{2m_y} + \frac{1 - \sqrt{\lambda} + 3\lambda + \lambda \sqrt{\lambda} |\Pi_x \Delta_d|^2}{(1+\sqrt{\lambda})^3} \frac{1}{2m_x} \right.
\]

\[
+ 1 + 3\sqrt{\lambda} - \lambda + \lambda \sqrt{\lambda} |\Pi_y \Delta_d|^2 \frac{1}{(1+\sqrt{\lambda})^3} \frac{1}{2m_y} \right]
\]

\[
+ \left(\frac{\lambda - 2\sqrt{\lambda} - 1 \Pi_x \Delta_s \Pi_x \Delta_d^*}{2m_x} - \frac{2\sqrt{\lambda} + 1 - \lambda \Pi_y \Delta_s \Pi_y \Delta_d^*}{2m_y} + \text{h.c.}\right)\right]
\]

\[
+ 2\gamma_d \alpha \left[\frac{(\lambda + 1)(1 + \sqrt{\lambda} + \lambda)}{(1 + \sqrt{\lambda})^4} |\Delta_d|^4 + \frac{1}{2} |\Delta_s|^4 + \frac{2(1+\lambda)}{(1+\sqrt{\lambda})^2} |\Delta_d|^2 |\Delta_s|^2 \right.
\]

\[
+ \frac{\lambda + 1}{2(1+\sqrt{\lambda})^2} (\Delta_s^2 \Delta_d^2 + \Delta_s^2 \Delta_d^2) + \frac{\sqrt{\lambda} - 1}{\sqrt{\lambda} + 1} |\Delta_s|^2 (\Delta_s^* \Delta_d + \Delta_s \Delta_d^*)
\]

\[
+ \frac{\lambda \sqrt{\lambda} - 1}{(1+\sqrt{\lambda})^3} |\Delta_d|^2 (\Delta_s^* \Delta_d + \Delta_s \Delta_d^*)\right].
\]

(2.13)

It is interesting to note in the above equation that except for the mixed gradient terms, which are induced by the magnetic field, there exist the new terms, such as

\[
\propto (\lambda - 1)(\Delta_s^* \Delta_d + \Delta_d^* \Delta_s)
\]

and

\[
\propto (\sqrt{\lambda} - 1) \left( |\Delta_s|^2 + \frac{1 + \sqrt{\lambda} + \lambda}{(1+\sqrt{\lambda})^2} |\Delta_d|^2 \right) (\Delta_s^* \Delta_d + \Delta_d^* \Delta_s).
\]

These new terms come completely from the mass anisotropy. For isotropic systems with $\lambda = 1$, these terms vanish. In the following section, we will discuss the physical consequences of these new terms.

**III. BULK SOLUTIONS**

In this section we study the solutions of the GL equations of an anisotropic $d$-wave superconductor for a bulk or uniform system. In this case the gradient terms in Eqs.(2.10) and (2.11) are equal to zero. First let us examine the $T_c$ formula. For $T \to T_c$, the coefficients of the linear terms in the GL equations determine the transition temperature:

\[
\ln \frac{T_c}{T_{c0}} = \frac{1}{\gamma_d} \left\{ 1 - \frac{(1+\sqrt{\lambda})^2}{2(1+\lambda)} \left[ 1 - \frac{1}{\alpha_s} \left( \frac{\lambda - 1}{\lambda + 1} \right)^2 \right] \right\},
\]

(3.1)
where $T_{c0}$ is the transition temperature for a purely $d$-wave superconductor corresponding to $\lambda = 1$, which is given by

$$\ln \frac{2e^\gamma \omega_D}{\pi T_{c0}} = \frac{1}{\gamma_d},$$

(3.2)

For a small anisotropy ($\lambda \rightarrow 1$), Eq.(3.1) reduces to

$$\ln \frac{T_c}{T_{c0}} = \frac{1}{4\gamma_d \alpha_s} (\lambda - 1)^2 > 0.$$  

(3.3)

This result implies that $T_c$ increases as the system deviates from the isotropy.

In the following discussion, for convenience, we put the GL free energy into a dimensionless form, which can be done by scaling the energy by $4\gamma_d(1 - T/T_c)^2/3\alpha$, lengths by $\xi_x = \sqrt{\mu\alpha/2m_x(1 - T/T_c)}$, and setting $\Delta_s = \psi_s \Delta_{d*}(\lambda = 1)$, $\Delta_d = \psi_d \Delta_{d*}(\lambda = 1)$, where $\Delta_{d*}(\lambda = 1) = \sqrt{4(1 - T/T_c)/3\alpha}$, and $A = (2\pi \xi_x/\Phi_0)A$:

$$F = - \frac{2(1 + \lambda)}{(1 + \sqrt{\lambda})^2} \left[ 1 - \frac{1}{\alpha_s \gamma_d(1 - T/T_c)} \left( \frac{\lambda - 1}{\lambda + 1} \right) \right] |\psi_d|^2 + \frac{\alpha_s}{\gamma_d(1 - T/T_c)} |\psi_s|^2$$

$$- \frac{1}{\gamma_d(1 - T/T_c)} \left( \frac{\lambda - 1}{\lambda + 1} \right) (\psi^*_s \psi_d + \psi^*_d \psi_s) + 2 \left( |\Pi_x \psi_s|^2 + \lambda |\Pi_y \psi_s|^2 \right)$$

$$+ 2 \left[ \frac{1 - \sqrt{\lambda}}{1 + \sqrt{\lambda}} |\Pi_x \psi_d|^2 + \lambda \frac{1 + 3 \sqrt{\lambda} - \lambda + \lambda \sqrt{\lambda}}{1 + \sqrt{\lambda}^3} |\Pi_y \psi_d|^2 \right]$$

$$+ 2 \left[ \frac{\lambda + 2 \sqrt{\lambda} - 1}{(1 + \sqrt{\lambda})^2} \Pi_x \psi_s \Pi_x \psi^*_d - \frac{1 + 2 \sqrt{\lambda} - \lambda}{(1 + \sqrt{\lambda})^2} \Pi_y \psi_s \Pi_y \psi^*_d + h.c. \right]$$

$$+ \frac{4}{3} \left( \frac{\lambda + 1}{1 + \sqrt{\lambda}} \right)^2 |\psi_d|^4 + \frac{4}{3} |\psi_s|^4 + \frac{16}{3} \frac{\lambda + 1}{1 + \sqrt{\lambda}} |\psi_d|^2 |\psi_s|^2$$

$$+ \frac{4}{3} \frac{\lambda + 1}{1 + \sqrt{\lambda}} \left( \psi^*_s \psi^*_d + \psi^*_d \psi^*_s \right) + \frac{8 \sqrt{\lambda} - 1}{3 \sqrt{\lambda} + 1} |\psi_s|^2 \left( \psi^*_s \psi_d + \psi^*_d \psi_s \right)$$

$$+ \frac{8 \lambda \sqrt{\lambda} - 1}{3 (1 + \sqrt{\lambda})^3} |\psi_d|^2 \left( \psi^*_s \psi_d + \psi^*_d \psi_s \right) + \kappa^2 (\nabla \times A)^2.$$  

(3.4)

In the above expression, the magnetic field energy has been included explicitly with $\kappa$ being the GL parameter. From $\delta F/\delta \psi_s^*$ and $\delta F/\delta \psi_d^*$ we can obtain the GL equations for $\psi_s$ and $\psi_d$. We now discuss the bulk solutions. Assuming $\psi_s = |\psi_s|e^{i\theta_s}$, $\psi_d = |\psi_d|e^{i\theta_d}$, and $\theta = \theta_s - \theta_d$, we can determine the value of $\theta$ through $\partial F/\partial \theta = 0$ and $\partial^2 F/\partial \theta^2 > 0$. We find that the stable solution is only possible for $\theta = 0$, which means that the bulk system is in the mixed $s + d$ state with a real combination. For $T \rightarrow T_c$, $\psi_s$ and $\psi_d$ are given by

$$\psi_s = \frac{1}{\alpha_s} \left( \frac{\lambda - 1}{\lambda + 1} \right) \psi_d,$$

(3.5)

$$\psi_d = D^{-1}(\lambda),$$  

(3.6)
with
\[ D(\lambda) = \frac{4}{3} \frac{(1 + \sqrt{\lambda})^2}{1 + \lambda} \left\{ \frac{(\lambda + 1)(\lambda + \sqrt{\lambda} + 1)}{(1 + \sqrt{\lambda})^4} + 2 \frac{\lambda \sqrt{\lambda} - 1}{(1 + \sqrt{\lambda})^3} \left( \frac{\lambda - 1}{\lambda + 1} \right) \frac{1}{\alpha_s} + \frac{3}{1 + \sqrt{\lambda}} \left( \frac{\lambda - 1}{\lambda + 1} \right)^2 \frac{1}{\alpha_s^2} + \frac{\sqrt{\lambda} - 1}{\sqrt{\lambda} + 1} \left( \frac{\lambda - 1}{\lambda + 1} \right)^3 \frac{1}{\alpha_s^4} \right\}. \] (3.7)

It is easy to see that \( D(\lambda) \to 1 \) as \( \lambda \to 1 \). Namely for an isotropic system with \( \lambda \to 1 \), \( \psi_d \to 1 \), and \( \psi_s \to 0 \), which implies that the purely \( d \)-wave state is only possible for the isotropic system. Whenever the system has an anisotropy, the mixed \( s+d \) state with \( \psi_d < 1 \) and \( \psi_s \neq 0 \) is generated. It is clear from Eq.(3.5) that these two order parameters have the same \( T_c \), which is given by Eq.(3.1). As argued by many authors \[9\], such a mixed \( s+d \) state in the bulk is just what we need to explain the tunneling data and other apparently conflicting results observed in YBCO.

IV. VORTEX SOLUTIONS

In this section, we determine the single vortex solutions for an anisotropic \( d \)-wave superconductor using the GL equations derived in Sec.II. Previously, we have studied the purely \( d \)-wave vortex structure \[9\] and found that near the vortex core, there coexist the \( s \)-wave and \( d \)-wave components with the opposite winding numbers. Far away from the vortex core, the induced \( s \)-wave component shows strong four-fold anisotropy and decays as \( r^{-2} \). We expect that the mass-anisotropy will affect the vortex structure. For simplification, here we study the case when \( \epsilon = \lambda - 1 \) is a small parameter. In this case the GL equations become

\[
\frac{\alpha_s}{\gamma_d(1-T/T_c)} \psi_s - \frac{\epsilon}{2\gamma(1-T/T_c)} \psi_d + \frac{8}{3} |\psi_s|^2 \psi_s + \frac{8}{3} |\psi_d|^2 \psi_s + \frac{4}{3} \psi_d \psi_s^* + \frac{2}{3} \epsilon (|\psi_d|^2 \psi_d + |\psi_s|^2 \psi_s) + \frac{1}{2} \epsilon |\psi_d|^2 \psi_d + 2 \Pi^2 \psi_s + (\Pi_x^2 - \Pi_y^2) \psi_d = 0, \tag{4.1}
\]

\[
- \psi_d + \frac{\epsilon^2}{4\alpha_s \gamma(1-T/T_c)} \psi_d - \frac{\epsilon}{2\gamma_d(1-T/T_c)} \psi_s + |\psi_d|^2 \psi_d + \frac{8}{3} |\psi_s|^2 \psi_d + \frac{4}{3} \psi_d \psi_s^* + \frac{2}{3} \epsilon |\psi_s|^2 \psi_s + \frac{1}{4} \epsilon (\psi_d^2 \psi_s^* + \psi_d \psi_s^2) + \Pi^2 \psi_d + (\Pi_x^2 - \Pi_y^2) \psi_s = 0. \tag{4.2}
\]

In terms of the cylindrical coordinates, \( R = (r, \theta) \), we expect that the \( d \)-wave component has the form \( \psi_d = e^{i\theta} \) in the region of \( 1 \ll r \ll \) London penetration depth. Also note that, in this region, the magnetic field effect can be neglected. Then the leading terms in the equation (4.1) for \( \psi_s \) are

\[
\frac{\alpha_s}{\gamma_d(1-T/T_c)} \psi_s - \frac{1}{2} \frac{\epsilon}{\gamma_d(1-T/T_c)} \left[ \frac{1}{\gamma_d(1-T/T_c)} - 1 \right] e^{i\theta} + \frac{8}{3} \psi_s + \frac{4}{3} e^{2i\theta} \psi_s - \left( \partial_x^2 - \partial_y^2 \right) e^{i\theta} = 0. \tag{4.3}
\]

This equation suggests the following solution:
\[ \psi_s = ae^{i\theta} + \frac{1}{r^2} (be^{-i\theta} - ce^{3i\theta}), \]  
(4.4)

where \[ a = \frac{3\tilde{\epsilon}(3\tilde{\alpha}_s + 4)}{(3\tilde{\alpha}_s + 8)^2 - 16}, \]  
(4.5)

\[ b = \frac{3}{2} \frac{3\tilde{\alpha}_s + 20}{(3\tilde{\alpha}_s + 8)^2 - 16}, \]  
(4.6)

\[ c = \frac{3}{2} \frac{9\tilde{\alpha}_s + 28}{(3\tilde{\alpha}_s + 8)^2 - 16}, \]  
(4.7)

with \[ \tilde{\alpha}_s = \frac{\alpha_s}{\gamma_d(1 - T/T_c)} \] and \[ \tilde{\epsilon} = \frac{1}{2}\epsilon [1/\gamma_d(1 - T/T_c) - 1]. \] For \( T \rightarrow T_c \), \( \psi_s \) takes the simple expression:

\[ \psi_s = \frac{\epsilon}{2\alpha_s} e^{i\theta} + \frac{\gamma_d(1 - T/T_c)}{2\alpha_s} \frac{1}{r^2} (e^{-i\theta} - 3e^{3i\theta}). \]  
(4.8)

It is very important to note that the first term in the above equation is independent of both temperature and the distance from the vortex core. This term comes, in fact, from the contribution of the bulk. Comparing this term with the bulk solution given in (3.4), we immediately find that they are identical for small \( \epsilon \) parameter. Our solution (4.4) implies that far away from the vortex core and the temperature approaches to \( T_c \), the bulk term of the \( s \)-wave component, with the same winding with respect to \( d \)-wave order parameter, becomes dominant. The magnitude of \( \psi_s \) is

\[ |\psi_s|^2 = a^2 + \frac{1}{r^4} (b^2 + c^2) + \frac{2a}{r^2} (b - c) \cos 2\theta - \frac{2bc}{r^4} \cos 4\theta. \]  
(4.9)

This result clearly shows a two-fold symmetry due to the existence of the \( \cos 2\theta \) term. If setting \( \epsilon = 0 \), the \( \cos 2\theta \) term vanishes, \( |\psi_s|^2 \) recovers the four-fold symmetry, and our result returns back to that for a purely \( d \)-wave superconductor, as given in Ref. [9].

Near the vortex core, to the leading order, our GL equations become

\[ -\psi_d - \nabla^2 \psi_d = 0, \]  
(4.10)

\[ \frac{\alpha_s}{\gamma_d(1 - T/T_c)} \psi_s - \frac{\epsilon}{2\gamma_d(1 - T/T_c)} \psi_d - 2\nabla^2 \psi_s - \left( \partial^2_x - \partial^2_y \right) \psi_d = 0. \]  
(4.11)

From (4.10) we have

\[ \psi_d = c_0 \left( r - \frac{1}{8} r^3 \right) e^{i\theta}, \]  
(4.12)

where \( c_0 \) is a constant. Putting the above equation into (4.11), we obtain
\[ \psi_s = \frac{\epsilon}{2\alpha_s}c_0re^{i\theta} - \frac{\gamma_d(1-T/T_c)}{2\alpha_s}c_0re^{-i\theta}. \quad (4.13) \]

Thus, the leading order terms of the order parameters near the vortex core are

\[ \psi_d = c_0re^{i\theta} \quad (4.14) \]
\[ \psi_s = \frac{\alpha_s}{2\alpha_s} \left[ \epsilon e^{i\theta} - \gamma_d(1-T/T_c)e^{-i\theta} \right]. \quad (4.15) \]

For isotropic systems with \( \epsilon = 0 \), the above results reduce to those for a purely \( d \)-wave superconductor. Namely, the \( s \)-wave component, with the opposite winding relative to the \( d \)-wave order parameter, is induced near the vortex core [9]. However, the anisotropy alters such a picture: As \( T \to T_c \), the opposite winding of the \( s \)-wave component is gradually taken over by the same winding term. Also \( e^{i\theta} \) and \( e^{-i\theta} \) terms in Eq.(4.15) combine to give a two-fold symmetry around the vortex core.

**V. NUMERICAL RESULTS OF SINGLE VORTEX**

In last section, we have discussed analytically the asymptotic behavior of the single vortex for an anisotropic \( d \)-wave superconductor. But the precise shape of the vortex structure is still not clear and it has to rely on the numerical calculation. Here, we perform a numerical study of the discretized GL free energy (3.4) using numerical relaxation approach [12][13]. In order to minimize the GL free energy functional in the presence of magnetic field, we use the constraint of fixing the average magnetic induction \( B \) by specifying the total flux \( \Phi \) in the unit cell, and impose the so-called “magnetic periodic boundary conditions” [13][14].

To perform the numerical relaxation calculation, we need to discretize the GL free energy (3.4) first. With the use of the forward difference approximation for the derivatives and taking into account the gauge invariance, we can write the free energy (3.4) in the discrete form:

\[ F = F_0 + F_{\text{kin}} + F_{\text{field}}, \quad (5.1) \]

where

\[
F_0 = \frac{1}{N_x N_y} \sum_{ij} \frac{2(1 + \lambda)}{(1 + \sqrt{\lambda})^2} \left[ 1 - \frac{1}{\alpha_s \gamma_d (1 - T/T_c)} \left( \frac{\lambda - 1}{\lambda + 1} \right) \right] |\psi_d(i, j)|^2 \\
+ \frac{\alpha_s}{\gamma_d (1 - T/T_c)} |\psi_s(i, j)|^2 - \frac{1}{\alpha_s \gamma_d (1 - T/T_c)} \left( \frac{\lambda - 1}{\lambda + 1} \right) \left[ \psi_s^*(i, j)\psi_d(i, j) + \psi_d^*(i, j)\psi_s(i, j) \right] \\
+ \frac{4}{3} \frac{(\lambda + 1)(\lambda + \sqrt{\lambda} + 1)}{(1 + \sqrt{\lambda})^4} |\psi_d(i, j)|^4 + \frac{4}{3} |\psi_s(i, j)|^4 + \frac{16}{3} \frac{\lambda + 1}{(1 + \sqrt{\lambda})^2} |\psi_d(i, j)|^2 |\psi_s(i, j)|^2 \\
+ \frac{4}{3} \frac{\lambda + 1}{(1 + \sqrt{\lambda})^2} \left[ \psi_s^2(i, j)\psi_d^2(i, j) + \psi_d^2(i, j)\psi_s^2(i, j) \right] \\
+ \frac{8}{3} \frac{\sqrt{\lambda} - 1}{\sqrt{\lambda} + 1} |\psi_d(i, j)|^2 \left[ \psi_s^*(i, j)\psi_d(i, j) + \psi_d^*(i, j)\psi_s(i, j) \right] \\
+ \frac{8}{3} \frac{\lambda \sqrt{\lambda} - 1}{(1 + \sqrt{\lambda})^3} |\psi_d(i, j)|^2 \left[ \psi_s^*(i, j)\psi_d(i, j) + \psi_d^*(i, j)\psi_s(i, j) \right], \quad (5.2)
\]
\[ F_{\text{kin}} = \frac{2}{N_x N_y} \sum_{ij} \left\{ \left| \psi_s(i+1,j) - \psi_s(i,j)e^{ia_x A_x(i,j)} \right|^2/a_x^2 \right. \\
+ \lambda \left| \psi_s(i,j+1) - \psi_s(i,j)e^{ia_y A_y(i,j)} \right|^2/a_y^2 \\
+ \frac{1 - \sqrt{\lambda} + 3\lambda + \lambda \sqrt{\lambda}}{(1 + \sqrt{\lambda})^3} \left| \psi_d(i+1,j) - \psi_d(i,j)e^{ia_x A_x(i,j)} \right|^2/a_x^2 \\
+ \frac{1 + 3\sqrt{\lambda} - \lambda + \lambda \sqrt{\lambda}}{(1 + \sqrt{\lambda})^3} \left| \psi_d(i,j+1) - \psi_d(i,j)e^{ia_y A_y(i,j)} \right|^2/a_y^2 \\
+ \left[ \frac{\lambda + 2\sqrt{\lambda} - 1}{(1 + \sqrt{\lambda})^2} \left( \psi_s(i+1,j) - \psi_s(i,j)e^{ia_x A_x(i,j)} \right) \\
\times \left( \psi_d^*(i+1,j) - \psi_d^*(i,j)e^{-ia_x A_x(i,j)} \right) \right] \left( \frac{\sqrt{\lambda} - 1}{(1 + \sqrt{\lambda})} \right)^2 \\
- \frac{2\sqrt{\lambda} + 1 - \lambda}{(1 + \sqrt{\lambda})^2} \left( \psi_s(i,j+1) - \psi_s(i,j)e^{ia_y A_y(i,j)} \right) \\
\times \left( \psi_d^*(i,j+1) - \psi_d^*(i,j)e^{-ia_y A_y(i,j)} \right) \right\}, \quad (5.3) \]

\[ F_{\text{field}} = \frac{\kappa^2}{N_x N_y} \sum_{ij} \left\{ \left[ A_y(i+1,j) - A_y(i,j) \right]/a_x - \left[ A_x(i,j+1) - A_x(i,j) \right]/a_y \right\}^2, \quad (5.4) \]

where \( N_x (N_y) \) is the number of lattice points in the \( x \) (\( y \)) direction. On each lattice point \((i, j)\), the order parameters \( \psi_s \) and \( \psi_d \) have the values \( \psi_s(i, j) \) and \( \psi_d(i, j) \), and each point is associated with horizontal and vertical bonds. \( a_x \) and \( a_y \) are the lattice constants and \( A_x(i, j) \) and \( A_y(i, j) \) are the vector potential components on bonds \([(i, j) \rightarrow (i+1, j)]\) and \([(i, j) \rightarrow (i, j+1)]\), respectively. It is easy to show that in these lattice notations, the above expressions are invariant with respect to gauge transformation:

\[
\psi_{s,d}(i,j) \rightarrow \psi_{s,d}(i,j)e^{i\chi(i,j)},
A_x(i,j) \rightarrow A_x(i,j) + [\chi(i+1,j) - \chi(i,j)]/a_x,
A_y(i,j) \rightarrow A_y(i,j) + [\chi(i,j+1) - \chi(i,j)]/a_y,
\]

where \( \chi(i,j) \) is the arbitrary phase of the order parameters at site \((i, j)\). Accordingly, the free energy and other physical quantities are also gauge invariant. To obtain simple boundary conditions we can choose a gauge such that \( A_x \) is independent of \( x \). In this case, our boundary conditions are \([14][13]\)

\[
A_x(0) = A_x(L_y), \quad (5.5)
A_y(L_x, y) - A_y(0, y) = \Phi/L_y, \quad (5.6)
A_y(x, L_y) = A_y(x, 0), \quad (5.7)
\psi_{s,d}(x, L_y) = \psi_{s,d}(x, 0)e^{i\Phi/2}, \quad (5.8)
\psi_{s,d}(L_x, y) = \psi_{s,d}(0, y)e^{i\Phi/L_y}, \quad (5.9)
\]

where \( L_x = N_x a_x \) and \( L_y = N_y a_y \). In order to study the single vortex structure, we can choose one quantum of flux (i.e., \( \Phi = 2\pi \)) in a square unit cell with \( N \times N \) lattice points.
With Eqs.(5.1)-(5.4) and the above boundary conditions, we can now realize the relaxation procedure. Choosing \( \psi_s, \psi_s^*, \psi_d, \psi_d^*, A_x, \) and \( A_y \) as independent variables, we can write down the relaxation iteration equations:

\[
\begin{align*}
\psi_s^{(n+1)}(i,j) &= \psi_s^{(n)}(i,j) - \epsilon_1 \frac{\partial F}{\partial \psi_s^*(i,j)} \\
\psi_d^{(n+1)}(i,j) &= \psi_d^{(n)}(i,j) - \epsilon_2 \frac{\partial F}{\partial \psi_d^*(i,j)} \\
A_x^{(n+1)}(i,j) &= A_x^{(n)}(i,j) - \epsilon_3 \frac{\partial F}{\partial A_x(i,j)} \\
A_y^{(n+1)}(i,j) &= A_y^{(n)}(i,j) - \epsilon_4 \frac{\partial F}{\partial A_y(i,j)}
\end{align*}
\]

where \( \epsilon \)'s are all positive numbers to be adjusted to optimize the convergence rate and \( n \) is an integer labeling the generations of iteration. It has been shown mathematically that \( F \) will monotonically decrease to its optimum state as \( n \) increases as long as we choose a proper initial state \([12]\).

In our numerical calculation, the parameters chosen are \( N_x = N_y = 101, a_x = a_y = 0.2\xi, \kappa = 2, T = 0.5T_c, \) and \( V_s = 0 \). With these parameters, the external magnetic field corresponds approximately to the thermal critical field \( H_c \). The use of the different parameters does not alter the qualitative physics. Let us first show the results for an isotropic \( d \)-wave vortex structure with \( \lambda = 1 \). Figs.1 and 2 are typical surface plots for the distribution of the \( d \)-wave order parameter and local magnetic field around the vortex, respectively, which look like the conventional \( s \)-wave vortex. But if looking at them closely, we find the difference from the conventional \( s \)-wave vortex. Fig.3 is the contour plot of the \( d \)-wave order parameter. It is clear that \(|\psi_d|\) exhibits a four-fold symmetry. The local magnetic field also shows a similar four-fold anisotropy (not shown in the contour plot).

The most interesting feature of a single vortex is that a small \( s \)-wave component is induced around the core, as shown in Fig.4 (A) (surface plot) and (B) (contour plot). One can clearly see that the distribution of \(|\psi_s|\) exhibits the profile in the shape of a four-leaved clover, which is in agreement with our analytical result \([7]\). We believe that the presence of this four-fold symmetric \( s \)-wave component is the reason to cause four-fold symmetry of the \( d \)-wave order parameter \(|\psi_d|\) (see Fig.3) and the local magnetic field \( h \) around the vortex.

We now discuss the anisotropic case with \( \lambda \neq 1 \). With the deviation of \( \lambda \) from unity, we find that both \(|\psi_d|\) and \( h \) begin to show a two-fold symmetry, in contrast to the four-fold symmetry as expected for a purely \( d \)-wave vortex. Specifically, both of them exhibit an elliptic shape. Fig.5 is the contour plot for \(|\psi_d|\) with \( \lambda = 2 \), which corresponds approximately to the measured penetration depth anisotropy \([3]\).

The \( s \)-wave component is much more sensitive to the anisotropic parameter \( \lambda \). Fig.6 (surface plot) and Fig.7 (contour plot) show how \(|\psi_s|\) changes with the increase of \( \lambda \). It is apparent that \(|\psi_s|\) exhibits the two-fold symmetry, and its shape changes from the four-leaved clover in the purely \( d \)-wave case \((\lambda = 1)\) to a butterfly as \( \lambda \) increases. These results agree well with our analytical calculation [see Eqs.(4.8) and (4.15)].

Recently, the vortex structure of YBCO has been directly observed using STM imaging technique \([7]\). An elongated shape of the vortex was realized. The ratio of the axes in
the apparent elliptic shape is about 1.5. Furthermore, this elongation was found to be independent of the scanning direction of the STM tip. We believe that this elongation directly reflects the $a$-$b$ anisotropy. This observed vortex shape can be qualitatively accounted for by the present GL theory for an anisotropic $d$-wave superconductor (see Fig.3).

VI. NUMERICAL RESULTS OF VORTEX LATTICE

Recent observation of an oblique vortex lattice structure in YBCO has been reported with the angle between the primitive axes $\beta \sim 73^0$ by the neutron scattering [16] and $\beta \sim 77^0$ by STM measurements [7]. The rich and complicated structure of a single vortex in an anisotropic $d$-wave superconductor obtained in the previous sections will be expected to form a different vortex lattice than the conventional $s$-wave superconductor, and may provide an explanation to the oblique vortex lattice structure observed in YBCO. To check this, the vortex lattice structure is going to be studied using numerical relaxation method.

The vortex lattice structure is still described by the discrete GL free energy functional given in Eqs.(5.1)-(5.4). We chose a rectangular unit cell with two vortices [14]. The periodic boundary conditions, very similar to Eqs.(5.5)-(5.9) except for $\Phi = 4\pi$ in the present case, are used in our calculations. The ratio of $a_y/a_x$ controls the shape of the vortex lattice structure. For example, $a_y/a_x = 1$ corresponds to the square, while $a_y/a_x = \sqrt{3}$ corresponds to triangular lattice. We have calculated the dependence of the free energy on the ratio of $a_y/a_x$ using the same set of parameters as for the single vortex.

Let us first present the results for the isotropic systems. Fig.8 displays the free energy as a function of $a_y/a_x$ for the isotropic $d$-wave superconductor ($\lambda = 1$). It is evident from the figure that the minimum of the free energy is at the position with $a_y/a_x \sim 1.3$, signaling that an oblique vortex lattice with the angle $\beta \sim 75^0$ between the primitive axes is stable. In this case, the superconducting state in the bulk or uniform system is purely $d$-wave. The $s$-wave component near the vortex core is induced due completely to the mixed gradient terms in the GL free energy. To correlate between the single vortex structure and the vortex lattice, we have performed the calculations for different temperatures. We find that in a wide temperature range below $T_c$, the presence of a sizable induced $s$-wave component causes four-fold symmetry of the $d$-wave order parameter and the local magnetic field around the vortex. Such an anisotropic single vortex tend to form an oblique lattice structure. Fig.9 shows the oblique vortex lattice formed at $T/T_c = 0.5$ by the $d$-wave order parameter (A) and the $s$-wave component (B) for the isotropic case ($\lambda = 1$). The local magnetic field distribution is very similar to the $d$-wave order parameter (not shown in the figure).

However, when $T \to T_c$, the induced $s$-wave component is strongly suppressed, which can be also seen from our analytical results given in Eqs.(4.8) and (4.13). In this case, the induced $s$-wave component is too small to affect the distribution of the $d$-wave order parameter and the local magnetic field. Consequently, both $\psi_d$ and $h$ have isotropic distribution around the vortex core, similar to the conventional $s$-wave vortex. These isotropic isolated vortices prefer to have a triangular vortex lattice, identical to the vortex lattice in an $s$-wave superconductor [15], as expected. This result is confirmed by our numerical calculation for the free energy that the minimum of the free energy moves to $a_y/a_x = \sqrt{3}$, i.e., the triangular lattice is stabilized.

We now turn to the anisotropic case. Recent STM measurements in YBCO revealed
an oblique vortex lattice with $\beta \sim 77^0$. Moreover, the elongated vortex cores with the ratio of principle axes about 1.5 were also found by this technique. As noted by the authors of Ref. [7], if this elongation reflects the intrinsic $a$-$b$ anisotropy in a conventional $s$-wave superconductor, such an anisotropy would lead to a distorted vortex lattice with an angle $\beta = 82^0$ inconsistent with the observed value. Thus it seems that the $a$-$b$ anisotropy alone can not explain the observed vortex lattice structure and additional effects, such as the order parameter symmetry, must be involved in order to account for the experimental data. We should note also that although the vortex lattice in a purely $d$-wave superconductor has an angle [10,17] very close to the observed value, the four-fold symmetric vortex cores obtained in this case are inconsistent with the observed elliptic vortex cores. In this regard, it is interesting to study the vortex lattice structure in an anisotropic $d$-wave superconductor which contains both the $a$-$b$ anisotropy as well as the $d$-wave order parameter symmetry. Fig.10 shows the free energy as a function of $a_y/a_x$ for $\lambda = 2$, which corresponds approximately to the experimental data on the penetration depth [3] and the coherence length [7]. It is clear that the minimum of the free energy locates at $a_y/a_x \sim 1.3$, almost the same position as for the isotropic $d$-wave superconductor.

We should mention that in an anisotropic $d$-wave superconductor, the $a$-$b$ anisotropy and the order parameter symmetry play very different roles in determining the vortex structures. The vortex tends to have a two-fold symmetry due to the $a$-$b$ anisotropy, while it tends to have a four-fold symmetry due to the $d$-wave pairing state. For small $\lambda$, the $d$-wave order parameter symmetry is important, and the anisotropy becomes dominant for large anisotropy, as long as the effect on the vortex structure is concerned. We would like to point out here that the similar oblique vortex lattice obtained in both isotropic ($\lambda = 1$) and anisotropic ($\lambda = 2$) $d$-wave superconductors is only a coincidence. In general, the real single vortex and the vortex lattice structures are determined by the competition between the anisotropy and the $d$-wave order parameter symmetry.

Fig.11 shows the vortex lattice formed by the $d$-wave (A) and $s$-wave (B) order parameters for an anisotropic $d$-wave superconductor with $\lambda = 2$. The local magnetic field distribution (not shown in the figure) is very similar to the $d$-wave component. It is seen that the vortex lattice is oblique with $\beta \sim 75^0$ and the vortex cores are elliptic. These results are in perfect agreement with the STM measurements on the vortex lattice structure in YBCO [7].

VII. CONCLUSIONS

We have established microscopically a GL theory for an anisotropic superconductor with $d_{x^2-y^2}$-wave pairing symmetry within the anisotropic effective mass approximation. The experimental basis of our model is recent measurements which revealed a large anisotropy of the penetration depth [3] and the coherence length [7] between $a$ and $b$ directions in YBCO due to the existence of the CuO chains. In our model, a single anisotropic parameter $\lambda$ is introduced which gives a measure of the difference in the two effective masses $m_x$ and $m_y$ and this parameter can be fitted to the measured penetration depth and the coherence length data. The GL equations obtained in the present work should be useful to study the various properties of YBCO.

We have considered the solution of the GL equations for a uniform or bulk system and found that the stable solution is the mixed $s + d$ state, and both the $s$- and $d$-wave order
parameters have the same transition temperature. Such an $s + d$ state is just what we need to explain the tunneling data \footnote{5} and the other apparently conflicting experimental data observed in YBCO.

We also solved the GL equations both analytically and numerically for the vortex structures. For the single vortex we find that the anisotropic $d$-wave vortex is very different from the purely $d$-wave case. Namely, both the $s$- and $d$-wave components show a two-fold symmetry, in contrast to the four-fold symmetry around the vortex as expected for the purely $d$-wave vortex. Specifically, the $d$-wave order parameter exhibits an elliptic shape and the $s$-wave component shows a shape of butterfly. With the deviation of $\lambda$ from unity, the opposite winding between the $s$- and $d$-wave components observed in the purely $d$-wave case is gradually taken over by the same winding number.

The vortex lattice is in general oblique for both the purely $d$-wave and the anisotropic $d$-wave superconductors. Although the angle between the primitive vectors of the vortex lattice in a purely $d$-wave superconductor is comparable to the observed value, the shape of the vortex cores are very different from the experiments. On the other hand, for an anisotropic $d$-wave superconductor, the shape of the vortex lattice is determined by the competition between the anisotropy and the $d$-wave order parameter symmetry. By using the anisotropic parameter obtained from the experimental data on the penetration depth and the coherence length, we were able to find a vortex lattice which agree well with experiments not only in angle between the primitive axes but also the elliptic shape of the vortex cores.

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FIGURES

Fig.1 Surface plot for the distribution of $|\psi_d|$ around a single vortex in the isotropic $d$-wave superconductor. The parameters used are given in the text.

Fig.2 Surface plot for the distribution of the local magnetic field $h$ around a single vortex in the isotropic $d$-wave superconductor.

Fig.3 Contour plot for the distribution of $|\psi_d|$ around a single vortex in the isotropic $d$-wave superconductor.

Fig.4 Distribution of $|\psi_s|$ around a single vortex in the isotropic $d$-wave superconductor. (A) Surface plot, and (B) contour plot.

Fig.5 Contour plot for the distribution of $|\psi_d|$ around a single vortex in the anisotropic $d$-wave superconductor with $\lambda = 2$.

Fig.6 Surface plot for the distribution of $|\psi_s|$ around a single vortex in the anisotropic $d$-wave superconductor with different anisotropic parameters: (A) $\lambda = 1.05$, (B) $\lambda = 1.2$, and (C) $\lambda = 2$.

Fig.7 Contour plot for the distribution of $|\psi_s|$ around a single vortex in the anisotropic $d$-wave superconductor with different anisotropic parameters: (A) $\lambda = 1.05$, (B) $\lambda = 1.2$, and (C) $\lambda = 2$.

Fig.8 Free energy as a function of the ratio of $a_y/a_x$ for vortex lattice in an isotropic $d$-wave superconductor.

Fig.9 Contour plots of the $d$- (A) and $s$-wave (B) order parameters for the stable vortex lattice structure in an isotropic $d$-wave superconductor with $a_y/a_x = 1.3$, corresponding to an oblique lattice with $\beta = 75^0$.

Fig.10 Free energy as a function of the ratio of $a_y/a_x$ for vortex lattice in an anisotropic $d$-wave superconductor with $\lambda = 2$.

Fig.11 Contour plots of the $d$- (A) and $s$-wave (B) order parameters for the stable vortex lattice structure in an isotropic $d$-wave superconductor ($\lambda = 2$) with $a_y/a_x = 1.3$, corresponding to an oblique lattice with $\beta = 75^0$. 