Ginzburg-Landau Equations and Vortex Structure of a $d_{x^2-y^2}$ Superconductor

Yong Ren, Ji-Hai Xu, and C. S. Ting
Texas Center for Superconductivity, University of Houston, Houston, Texas 77204
(Received 2 December 1995)

We derive microscopically the Ginzburg-Landau equations of a superconductor with $d_{x^2-y^2}$ symmetry. The structure of a single vortex in such a superconductor is determined by solving these equations. The most interesting feature of the vortex structure is the opposite winding s-wave component induced near the vortex core. Far away from the center of the vortex core, the winding of the s-wave component becomes more complicated and the magnitude shows strong anisotropy. The distributions of supercurrent and local magnetic field also show anisotropic behaviors.

PACS numbers: 74.60.Ec, 74.72.–h

Recently both theories and experiments have suggested that the high T_c superconductors might possess unconventional pairing symmetry [1–3]. The vortex structure of a superconductor with $d_{x^2-y^2}$ pairing symmetry is of great interest because it might be relevant to high T_c superconductors [2]. It is expected that the structure of a d-wave vortex is very different from that of s wave [4,5] or p wave [6]. In particular, the detailed structure might be helpful for a theory to reconcile with experiments on transport properties in the mixed state [7]. Volovik [8] is the first one who studied the density of states of a d-wave vortex core. Based on symmetry considerations, he argues that the core of the vortex in the d-wave superconductor should contain all the possible gap functions that are consistent with the maximal symmetry group of the vortex line. In particular, it should contain the amplitude of the conventional s-wave pairing with the opposite winding phase. Because of this correction, the total gap function has no lines of gap nodes within the core. Soininen, Kallin, and Berlinsky [9] calculated the vortex structure numerically on a 16×16 lattice within the framework of the self-consistent Bogoliubov–de Gennes theory. They identified three different regions of the vortex; far away from the center a pure d wave exists, and near the center there is a normal "inner core" where both s wave and d wave vanish; in the middle region d wave and s wave coexist. However, due to its numerical nature, the behavior of each component is not clear from their calculations, and the approximate size of each region cannot be determined. They are also unable to study the temperature (T) dependence of the order parameters.

In this Letter, we derive the Ginzburg-Landau equations for a d-wave superconductor by using the finite temperature Green's function method. To this end, we begin with the Gor'kov equations [10]

$$\left\{i\omega_n - \frac{1}{2m}(-i\nabla + e\mathbf{A})^2 + \mu\right\}\tilde{G}(\mathbf{x},\mathbf{x}',\omega_n) + \int d\mathbf{x}''\,\Delta(\mathbf{x},\mathbf{x}'')F^+(\mathbf{x}'',\mathbf{x}',\omega_n) = \delta(\mathbf{x}-\mathbf{x}'), \tag{1}$$

$$\left\{-i\omega_n - \frac{1}{2m}(i\nabla + e\mathbf{A})^2 + \mu\right\}F^+(\mathbf{x},\mathbf{x}',\omega_n) + \int d\mathbf{x}''\,\Delta^*(\mathbf{x},\mathbf{x}'')\tilde{G}(\mathbf{x}'',\mathbf{x}',\omega_n) = 0, \tag{2}$$

and derive equations for the $\mathbf{k}$ dependence of the order parameter. Here $\tilde{G}$ and F are, respectively, the single particle and pair propagators. $\omega_n = (2n+1)\pi T$. By definition, the order parameter in real space is

$$\Delta^*(\mathbf{x},\mathbf{x}') = V(\mathbf{x}-\mathbf{x}')T\sum_{\omega_n} F^\dagger(\mathbf{x},\mathbf{x}',\omega_n), \tag{3}$$

with $-V(\mathbf{x}-\mathbf{x}')$ as the effective pairing interaction between two charge carriers. From Eqs. (1) and (2), and iterating Eq. (3) to the third order in Δ, we find

$$\Delta^*(\mathbf{x},\mathbf{y}) = V(\mathbf{x}-\mathbf{y})T\sum_{\omega_n}\bigg\{\int d\mathbf{x}'\,d\mathbf{x}''\,\tilde{G}_0(\mathbf{x}',\mathbf{x},-\omega_n)\Delta^*(\mathbf{x}',\mathbf{x}'')\bigg[\tilde{G}_0(\mathbf{x}'',\mathbf{y},\omega_n) - \int d\mathbf{x}_1\,d\mathbf{x}_2\,\tilde{G}_0(\mathbf{x}'',\mathbf{x}_1,\omega_n)\Delta(\mathbf{x}_1,\mathbf{x}_2)\int d\mathbf{x}_3\,d\mathbf{x}_4\,\tilde{G}_0(\mathbf{x}_3,\mathbf{x}_2,-\omega_n)\Delta^*(\mathbf{x}_3,\mathbf{x}_4)\tilde{G}_0(\mathbf{x}_4,\mathbf{y},\omega_n)\bigg]\bigg\}, \tag{4}$$

where $\tilde{G}_0$ is the Green's function of free electrons in magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$. In the case that we are interested in where $1/k_F$ (k_F is the Fermi wave number) is much less than the London penetration depth, $\tilde{G}_0$ can be related to the zero field Green's function G_0 via the approximate expression [11]

$$\tilde{G}_0(\mathbf{x},\mathbf{x}',\omega_n) \approx G_0(\mathbf{x}-\mathbf{x}',\omega_n)e^{-ie\mathbf{A}(\mathbf{x})\cdot(\mathbf{x}-\mathbf{x}')}, \tag{5}$$

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and

$$G_0(\mathbf{x},\omega_n) = \frac{1}{(2\pi)^2}\int d\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{x}} \frac{1}{i\omega_n - \xi_{\mathbf{k}}}, \tag{6}$$

where $\xi_{\mathbf{k}} = (\mathbf{k}^2/2m) - \mu$ is the kinetic energy of the charge carrier with mass m measured from the chemical potential μ. And we have assumed the Fermi surface is two dimensional as in the case of high T_c superconductors. Employing the approximation

$$\Delta^*(\mathbf{x}',\mathbf{x}'') \approx e^{\int_x^{x'} \nabla_x\cdot d\mathbf{l} + \int_y^{x''} \nabla_y \cdot d\mathbf{l}} \Delta^*(\mathbf{x},\mathbf{y}), \tag{7}$$

and rewriting everything in terms of the center of mass coordinates $\mathbf{R} = \frac{1}{2}(\mathbf{x}+\mathbf{y}), \mathbf{R}' = \frac{1}{2}(\mathbf{x}'+\mathbf{x}'')$ and the relative coordinates $\mathbf{r} = \mathbf{x} - \mathbf{y}, \mathbf{r}' = \mathbf{x}' - \mathbf{x}''$, the first term of Δ^* in Eq. (4) can be written as

$$\Delta^*_{(1)}(\mathbf{R},\mathbf{r}) = V(\mathbf{r})\int d\mathbf{R}\, d\mathbf{r}'\, T\sum_{\omega_n} G_0\Big(\mathbf{R}' + \frac{\mathbf{r}'}{2} - \mathbf{R} - \frac{\mathbf{r}}{2}, -\omega_n\Big) G_0\Big(\mathbf{R}' - \frac{\mathbf{r}'}{2} - \mathbf{R} + \frac{\mathbf{r}}{2}, \omega_n\Big) \times e^{i(\mathbf{R}'-\mathbf{R})\cdot(-i\nabla_{\mathbf{R}} - 2eA_{\mathbf{R}}) + i(\mathbf{r}'-\mathbf{r})\cdot(-i\nabla_{\mathbf{r}})} \Delta^*(\mathbf{R},\mathbf{r}). \tag{8}$$

In the above equation we have assumed the slow variation of magnetic field $A(\mathbf{x}) \approx A(\mathbf{y}) = A_{\mathbf{R}}$ or that the magnetic field acts only on the center of mass of the Cooper pair, not on the relative coordinate.

Expanding in terms of $\Pi = -i\nabla_{\mathbf{R}} - 2eA_{\mathbf{R}}$ to second order, and performing the Fourier transform with respect to the relative coordinate, Eq. (8) becomes

$$\Delta^*_{(1)}(\mathbf{R},\mathbf{k}) = \int \frac{d\mathbf{k}'}{(2\pi)^2} V(\mathbf{k}' - \mathbf{k}) \Big\{ T\sum_{\omega_n} \frac{1}{\omega_n^2 + \xi_{\mathbf{k}'^2}} + \frac{T}{2}\sum_{\omega_n}\Big[\frac{1}{(2m)^2}\frac{2\xi_{\mathbf{k}'}^2 - 6\omega_n^2}{(\omega_n^2 + \xi_{\mathbf{k}'}^2)^3}(k_x'^2\Pi_x^2 + k_y'^2\Pi_y^2) - \frac{1}{2m}\frac{\xi_{\mathbf{k}'}}{(\omega_n^2+\xi_{\mathbf{k}'}^2)^2}\Pi^2\Big]\Big\}\Delta^*(\mathbf{R},\mathbf{k}'). \tag{9}$$

Neglecting the contribution from the vector potential $\mathbf{A}$ [11], the remaining term of Δ in Eq. (4) takes the expression

$$\Delta^*_{(2)}(\mathbf{R},\mathbf{k}) = -\int \frac{d\mathbf{k}'}{(2\pi)^2} V(\mathbf{k} - \mathbf{k}') T\sum_{\omega_n}\frac{1}{(\omega_n^2 + \xi_{\mathbf{k}'}^2)^2} \times |\Delta^*(\mathbf{R},\mathbf{k}')|^2 \Delta^*(\mathbf{R},\mathbf{k}'). \tag{10}$$

According to Eq. (4) $\Delta^*_{(1)}(\mathbf{R},\mathbf{k}) + \Delta^*_{(2)}(\mathbf{R},\mathbf{k}) = \Delta^*(\mathbf{R},\mathbf{k})$. To obtain the generic Ginzburg-Landau equation for a d-wave superconductor, we make the following ansatz [12]:

$$V(\mathbf{k} - \mathbf{k}') = -V_s + V_d(\hat{k}_x^2 - \hat{k}_y^2)(\hat{k}_x'^2 - \hat{k}_y'^2), \tag{11}$$

$$\Delta^*(\mathbf{R},\mathbf{k}) = \Delta_s^*(\mathbf{R}) + \Delta_d^*(\mathbf{R})(\hat{k}_x^2 - \hat{k}_y^2), \tag{12}$$

where $\hat{\mathbf{k}}$ is the unit vector in the direction of $\mathbf{k}$. By taking both V_d and V_s positive, then $-V_d$ corresponds to the attractive interaction responsible for d-wave pairing and V_s represents a repulsive "on-site" interaction.

From Eqs. (9) and (10) and comparing both sides of $\Delta^*_{(1)}(\mathbf{R},\mathbf{k}) + \Delta^*_{(2)}(\mathbf{R},\mathbf{k}) = \Delta^*(\mathbf{R},\mathbf{k})$ for $\hat{k}$-independent terms and terms proportional to $(\hat{k}_x^2 - \hat{k}_y^2)$, we obtain

$$\Delta_s^* = -N(0)V_s\Delta_s^* \ln\frac{2e^\gamma \omega_D}{\pi T} + \frac{7\zeta(3)}{8}\frac{1}{(\pi T)^2}N(0)V_s \times \Big\{\frac{1}{4}v_F^2\Pi^2\Delta_s^* + \frac{1}{8}v_F^2(\Pi_x^2 - \Pi_y^2)\Delta_d^* + |\Delta_s|^2\Delta_s^* + |\Delta_d|^2\Delta_s^* + \frac{1}{2}\Delta_d^{*2}\Delta_s\Big\}, \tag{13}$$

$$\Delta_d^* = \frac{1}{2}N(0)V_d\Delta_d^* \ln\frac{2e^\gamma\omega_D}{\pi T} - \frac{7\zeta(3)}{8}\frac{1}{(\pi T)^2}N(0)V_d \times \Big\{\frac{1}{8}v_F^2\Pi^2\Delta_d^* + \frac{1}{8}v_F^2(\Pi_x^2 - \Pi_y^2)\Delta_s^* + |\Delta_s|^2\Delta_d^* + \frac{1}{2}\Delta_s^{*2}\Delta_d + \frac{3}{8}|\Delta_d|^2\Delta_d^*\Big\}. \tag{14}$$

Here γ is the Euler constant, $N(0)$ is the density of states at the Fermi surface, v_F is the Fermi velocity, and ω_D is the cutoff frequency for the interactions. A closer examination shows that Eq. (13) will lead to unphysical solutions for Δ_s, because its convergency is not established. To avoid this difficulty, we employ the Padé approximation,

$$\Delta_s^* \approx -2g_0\Delta_s^*\Big\{1 + \frac{\alpha\lambda_d}{\Delta_s^*}\Big[\frac{1}{4}v_F^2\Pi^2\Delta_s^* + \frac{1}{8}v_F^2(\Pi_x^2 - \Pi_y^2)\Delta_d^* + |\Delta_s|^2\Delta_s^* + |\Delta_d|^2\Delta_s^* + \frac{1}{2}\Delta_d^{*2}\Delta_s\Big]\Big\}^{-1}, \tag{15}$$

with $g_0 = V_s/V_d$, $\alpha = 7\zeta(3)/8(\pi T)^2$, and $\lambda_d = \frac{1}{2}N(0)V_d$.

The free energy obtained from the above equations is

$$f = 2(1 + 2g_0)|\Delta_s|^2 - \lambda_d \ln(T_c/T)|\Delta_d|^2 + \alpha\lambda_d[|\Delta_s|^4 + \tfrac{3}{8}|\Delta_d|^4 + 2|\Delta_s|^2|\Delta_d|^2 + \tfrac{1}{2}(\Delta_s^{*2}\Delta_d^2 + \Delta_d^{*2}\Delta_s^2)] + \tfrac{1}{4}\alpha\lambda_d v_F^2[2|\Pi\Delta_s^*|^2 + |\Pi\Delta_d^*|^2 + (\Pi_x^*\Delta_s\Pi_x\Delta_d^* - \Pi_y^*\Delta_s\Pi_y\Delta_d^* + \text{H.c.})]. \tag{16}$$

The corresponding expression for the current can be obtained from Gor'kov's equations,

$$\mathbf{j}(\mathbf{R}) = \frac{e\alpha N(0)E_F}{2m}\left[\Delta_s^*\mathbf{\Pi}^*\Delta_s + \frac{1}{2}\Delta_d^*\mathbf{\Pi}^*\Delta_d + \frac{1}{2}(\Delta_s^*\Pi_x^*\Delta_d + \Delta_d^*\Pi_x^*\Delta_s)\hat{\mathbf{x}} - \frac{1}{2}(\Delta_s^*\Pi_y^*\Delta_d + \Delta_d^*\Pi_y^*\Delta_s)\hat{\mathbf{y}}\right] + \text{H.c.} \tag{17}$$

Since the coefficients $2(1 + 2g_0) > 0$ and $-\ln(T_c/T) < 0$, it is easily seen that the pure d-wave solution is stable at infinity, as expected. At the first glance, the $\Delta_s^{*2}\Delta_d^2$ term favors a relative phase $\pi/2$ between s-wave and d-wave order parameters, or $s + id$ symmetry, but we shall show in the following discussion that the presence of the mixed gradient term alters such a picture. To study the structure of a single vortex when the coherence length is much smaller than the penetration depth, we define $\xi_0 = \sqrt{\alpha}\, v_F/2$ which differs from the usual coherence length at zero temperature only by a numerical factor ~ 1 and $\Delta_0 = \sqrt{4/3\alpha}$, and cast the Ginzburg-Landau equations into dimensionless form $r/\xi_0 \longrightarrow r$, $\Delta/\Delta_0 \longrightarrow \Delta$,

$$\alpha_s\Delta_s^* + \Pi^2\Delta_s^* + \frac{1}{2}(\Pi_x^2 - \Pi_y^2)\Delta_d^* + \frac{4}{3}|\Delta_s|^2\Delta_s^* + \frac{4}{3}|\Delta_d|^2\Delta_s^* + \frac{2}{3}\Delta_d^{*2}\Delta_s = 0, \tag{18}$$

$$-\ln(T_c/T)\Delta_d^* + \Pi^2\Delta_d^* + (\Pi_x^2 - \Pi_y^2)\Delta_s^* + \frac{8}{3}|\Delta_s|^2\Delta_d^* + \frac{4}{3}\Delta_s^{*2}\Delta_d + |\Delta_d|^2\Delta_d^* = 0, \tag{19}$$

where $\alpha_s = (1 + 2g_0)/\lambda_d$.

In terms of cylindrical coordinates, $\mathbf{R} = (r, \theta)$, we expect that, far away from the center of the vortex, the d-wave order parameter in the gauge choice $\mathbf{A}_\infty = \hat{\boldsymbol{\theta}}/2er$ takes the form $\Delta_d^* = e^{i\theta}g(r)$. Simple inspection of the Ginzburg-Landau equation shows that the leading order terms that are important at large distances are

$$\alpha_s\Delta_s^* + \tfrac{1}{2}(\Pi_x^2 - \Pi_y^2)ge^{i\theta} + \tfrac{4}{3}g^2\Delta_s^* + \tfrac{2}{3}g^2e^{2i\theta}\Delta_s = 0, \tag{20}$$

$$-\ln(T_c/T)g + g^3 = 0, \tag{21}$$

$$\nabla^2\mathbf{A} = \frac{1}{\lambda^2}\left(\mathbf{A} - \frac{1}{2er}\hat{\boldsymbol{\theta}}\right)^2 g^2, \quad \lambda^2 = 3m/8\pi ne^2. \tag{22}$$

Equation (20) suggests that the solution for Δ_s^* has the form $\Delta_s^* = (-ae^{-i\theta} + be^{3i\theta})/r^2$. In the physically interesting region $\xi \ll r \ll \lambda$, Eqs. (20) and (21) are easily solved to give

$$g(r) = [\ln(T_c/T)]^{1/2}, \tag{23}$$

$$a = \left[\left(\alpha_s + \frac{4}{3}g^2\right)^2 - \left(\frac{2}{3}g^2\right)^2\right]^{-1}\left[\alpha_s + \frac{10}{3}g^2\right]\frac{g}{4}, \tag{24}$$

$$b = \left[\left(\alpha_s + \frac{4}{3}g^2\right)^2 - \left(\frac{2}{3}g^2\right)^2\right]^{-1}\left[3\alpha_s + \frac{14}{3}g^2\right]\frac{g}{4}. \tag{25}$$

Thus the induced s-wave component decays as $1/r^2$ far away from the core and the $e^{-i\theta}$ and $e^{3i\theta}$ terms combine to give the profile the shape of a four-leafed clover (see Fig. 1).

Near the center of the vortex, to the leading order, our Ginzburg-Landau equations become

$$\Pi^2\Delta_d^* + (\Pi_x^2 - \Pi_y^2)\Delta_s^* = 0, \tag{26}$$

$$\Pi^2\Delta_s^* + \frac{1}{2}(\Pi_x^2 - \Pi_y^2)\Delta_d^* = 0. \tag{27}$$

The solution again has the form $\Delta_d^* = g(r)e^{i\theta}$, $\Delta_s^* = f_1(r)e^{-i\theta} + f_2(r)e^{3i\theta}$.

The general solutions to Eqs. (26) and (27) are $f_1(r) = c_1r$, $g(r) = c_0r$, and to the same order $f_2(r) = 0$. So, near the center of the core, $\Delta_d^* \sim c_0re^{i\theta}$, $\Delta_s^* \sim c_1re^{-i\theta}$, where the constants c_0 and c_1 have to be determined by connecting the solution near the center with the solution far away from the core, just as in the case of a conventional s-wave vortex [4]. Thus near the center of the vortex the s wave has the opposite winding number relative to the d-wave component [8]. This kind of mixing of s-wave and d-wave components is different from what has been studied before [13]. The relative phase between s-wave and d-wave components is shown in Fig. 2 for both far from and near the center of the vortex. In general, the full solution to the Ginzburg-Landau equations of a single vortex involves all possible terms that are consistent with the maximal symmetry group of the vortex: $\Delta_d^* = \sum_n g_n(r)e^{i(4n+1)\theta}$ and $\Delta_s^* = \sum_m f_m(r)e^{i(4m-1)\theta}$, where n, m need to be summed over all integers. The immediate consequence of the coexistence of s-wave and d-wave pairing is that there will be no lines of gap nodes within the core, so fermionic excitations will be gapped.

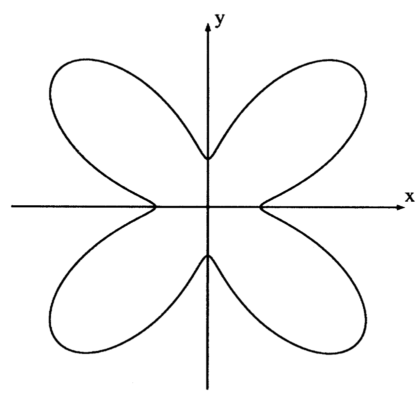

FIG. 1. The magnitude of s-wave component $|\Delta_s|^2$ far away from the core. The profile has the shape of a four-leafed clover.

It is interesting to note that the s-wave component is suppressed by V_s, which should correspond to the on-site repulsion used in Ref. [9]. On the other hand, our calculation shows that even when $V_s \longrightarrow 0$ the s-wave component still persists. The characteristic decaying length of the s-wave order parameter measured from the center of the vortex core is $\xi_0/\sqrt{\alpha_s}$, which is also suppressed by V_s. The temperature dependence of the s-wave order parameter is complicated, but near the transition temperature it has the same behavior as the d-wave component, namely, $[1 - (T/T_c)]^{1/2}$.

To calculate the supercurrent and local magnetic field, we need to consider the $1/r^2$ order corrections to Δ_d^* when $\xi \ll r \ll \lambda$, which turns out to consist of terms proportional to $e^{i\theta}$, $e^{5i\theta}$, and $e^{-3i\theta}$, respectively. We obtain, for $r \longrightarrow 0$,

$$\mathbf{j} = \tfrac{1}{2}(c_0^2 + 2c_1^2)r\hat{\boldsymbol{\theta}}, \tag{28}$$

$$\mathbf{B} = [B_0 - \tfrac{1}{4}(c_0^2 + 2c_1^2)r^2]\hat{\mathbf{z}}, \tag{29}$$

and for $\xi \ll r \ll \lambda$,

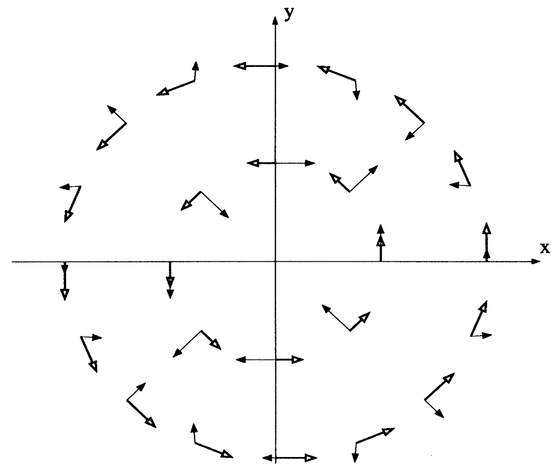

FIG. 2. The relative phase between s-wave and d-wave components. The vectors with the outlined arrow represent the d-wave order parameter, while the vectors with filled arrow represent the s-wave. The angle between the two vectors is the relative phase. We have only drawn the cases near the center of the vortex and far away from the core.

$$\mathbf{j} = \frac{\Phi_0 g^2}{2\pi\lambda^2}\left\{\frac{2(a+3b)}{r^3}\sin 4\theta\hat{\mathbf{r}} - \left[\frac{1}{r} + \frac{1}{g^2r^3} + \frac{a-b}{r^3} + \frac{a+3b}{r^3}\cos 4\theta\right]\hat{\boldsymbol{\theta}}\right\}, \tag{30}$$

$$\mathbf{B} = \Phi_0\frac{g^2}{2\pi\lambda^2}\hat{\mathbf{z}}\left[\ln\frac{\lambda}{r} - 2 - \frac{1}{g^2r^2} - \frac{a-b}{r^2} - \frac{a+3b}{2r^2}\cos 4\theta\right], \tag{31}$$

where $\Phi_0 = h/2e$ is the flux quantum. Such an anisotropic distribution could be measured in principle by methods such as the scanning SQUIDs [3].

In summary, we have derived microscopically the Ginzburg-Landau equations for a $d_{x^2-y^2}$ superconductor, and obtained the asymptotic behavior of the single vortex structure. Such a structure could be observed in scanning tunneling microscopy on d-wave superconductors. This is the first time that an analytical approach to the d-wave vortex structure has been constructed. The Ginzburg-Landau equations that we obtained should provide a convenient starting point for studying various properties of the superconducting state in a d-wave superconductor.

We would like to thank Professor F.C. Zhang and Professor T.K. Lee for helpful discussions. This research was supported by the State of Texas through the Texas Center for Superconductivity at the University of Houston, the Texas Advanced Research Program, and the Robert A. Welch Foundation.

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