Ginzburg-Landau Theory of Vortices in *d*-Wave Superconductors

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Ginzburg-Landau theory is used to study the properties of single vortices and of the Abrikosov vortex lattice in a $d_{x^2-y^2}$ superconductor. For a single vortex, the s-wave order parameter has the expected four-lobe structure in a ring around the core and falls off like $1/r^2$ at large distances. The topological structure of the s-wave order parameter consists of one counterrotating unit vortex, centered at the core, surrounded by four symmetrically placed positive unit vortices. The Abrikosov lattice varies continuously from triangular, through oblique, to square with increasing field and s-d mixing parameter ϵ_v. Comparison is made to recent neutron scattering data.

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Despite nearly a decade of intense experimental and theoretical activity, the nature of the microscopic mechanism for high T_c superconductivity remains controversial. Nevertheless, there has been considerable recent progress in understanding the phenomenology of these materials. For example, it seems clear that some sort of Cooper pairing is required to explain various observations, and there is mounting evidence for the existence of nodes with d-wave symmetry in the energy gap at the Fermi surface [1], which provides a strong incentive for studying the phenomenology of superconductors with such gap structures. As in the somewhat analogous case of superfluid ^{3}He, these questions are most pressing for a superfluid with a nonuniform condensate. Here we consider the behavior of a d-wave superconductor in a uniform magnetic field. The resulting quantized vortices exhibit a novel and complex structure, both individually and collectively when they form a dense lattice, particularly because of the presence of an induced s-wave component that would be absent in a strictly uniform system. These effects are likely to play a significant role in the transport properties of high T_c superconductors.

We have previously considered [2] a simple microscopic model of d-wave superconductivity for electrons on a lattice and used the Bogoliubov–de Gennes equations to calculate the order parameter distribution for a single vortex. The relevant Ginzburg-Landau (GL) free energy [3] served to interpret our results. Conversely, our microscopic results demonstrated the value of this GL model. The GL theory involves both the d-wave order parameter and an induced s-wave order parameter which arises in inhomogeneous states through a mixed gradient coupling [3–5].

Experience with conventional (s-wave) superconductors has demonstrated that virtually all of their phenomenological properties can be derived from the appropriate GL theory. The purpose of this paper is to develop the analogous GL theory for a $d_{x^2-y^2}$ superconductor based on the insights obtained from the microscopic model [2]. First, we investigate the structure of a single vortex near $H_{c1}(T)$. Our main result is that the s-wave component of the order parameter exhibits a nontrivial internal topological structure, shown in Fig. 1. Second, we solve for the structure of the vortex lattice close to $H_{c2}(T)$, by first minimizing the quadratic part of the free energy using a simple variational wave function and then forming a periodic array of vortices from linear combinations of these functions. The results are compared to recent small angle neutron scattering (SANS) data [6].

The free energy of a $d_{x^2-y^2}$ superconductor may be expressed in terms of the two order parameters $s(\mathbf{r})$ and $d(\mathbf{r})$ with appropriate symmetries as follows [2,3]:

$$\begin{aligned} f = {} & \alpha_s|s|^2 + \alpha_d|d|^2 + \beta_1|s|^4 + \beta_2|d|^4 \\ & + \beta_3|s|^2|d|^2 + \beta_4(s^{*2}d^2 + d^{*2}s^2) \\ & + \gamma_s|\mathbf{\Pi}s|^2 + \gamma_d|\mathbf{\Pi}d|^2 \\ & + \gamma_v[(\Pi_y s)^*(\Pi_y d) - (\Pi_x s)^*(\Pi_x d) + \text{c.c.}]\,. \end{aligned} \quad (1)$$

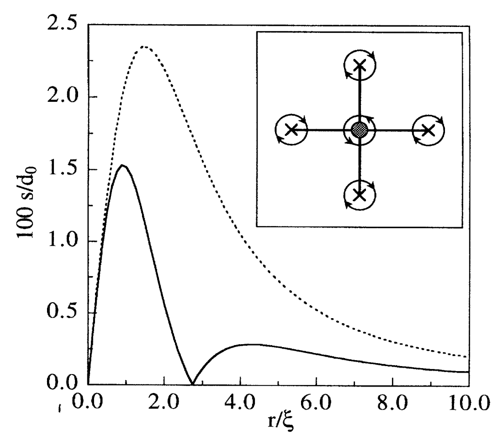

FIG. 1. Amplitude of the s-wave component along the x axis (solid line) and along the diagonal $x = y$ (dotted line) normalized to the bulk value d_0. The parameters used are $\gamma_s = \gamma_d = \gamma_v$, $\alpha_s = 10|\alpha_d|$, $\beta_1 = \beta_3 = 0$, and $\beta_4 = 0.5\beta_2$. The inset shows schematically the positions of the s-wave vortices and their relative windings.

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Here $\mathbf{\Pi} = -i\nabla - e^*\mathbf{A}/c\hbar$, and d is assumed to be the critical order parameter, i.e., we take $\alpha_s = T - T_s$ and $\alpha_d = T - T_d$ with $T_s < T_d$. The temperature derivatives of α_s and α_d are equal by tetragonal symmetry and have been arbitrarily set equal to 1. It is also assumed that β_1, β_2, β_3, β_4, γ_s, γ_d, and γ_v are all positive [2]. The parameters γ_i are related to the effective masses in the usual way, with $\gamma_i = \hbar^2/2m_i^*$, for $i = s, d, v$. For a stable $d_{x^2-y^2}$ superconductor one expects T_s to lie well below T_d, and, when $|d| > 0$, the tendency for $|s|$ to become nonzero is suppressed even further by the $\beta_3|s|^2|d|^2$ term. However, as was shown numerically in Ref. [2] and analytically in Ref. [7], a substantial mixed gradient term (γ_v) occurs in BCS-like mean field theories of $d_{x^2-y^2}$ superconductivity. This term implies that $|s| > 0$ whenever $|\nabla d| \neq 0$, even for $T_s \ll T$. The field equations for the order parameters are obtained by varying the free energy (1) with respect to conjugate fields d^* and s^*, giving

$$
\begin{aligned}
(\gamma_d \Pi^2 + \alpha_d)d + \gamma_v(\Pi_y^2 - \Pi_x^2)s + 2\beta_2|d|^2 d + \beta_3|s|^2 d + 2\beta_4 s^2 d^* &= 0, \\
(\gamma_s \Pi^2 + \alpha_s)s + \gamma_v(\Pi_y^2 - \Pi_x^2)d + 2\beta_1|s|^2 s + \beta_3|d|^2 s + 2\beta_4 d^2 s^* &= 0.
\end{aligned}
\tag{2}
$$

Equations (2) can be integrated numerically for boundary conditions which generate a single vortex at the origin. In doing this, we assume an extreme type-II limit, where the coupling to the vector potential can be ignored while considering the core structure of the isolated vortex line.

Ren, Xu, and Ting [7] have previously shown that for a d-wave order parameter with the asymptotic form

$$d(r,\theta) = d_0 e^{i\theta}, \tag{3}$$

where $d_0 = \sqrt{-\alpha_d/2\beta_2}$, the asymptotic form of the s-wave order parameter is

$$s(r,\theta) = g_1(r)e^{-i\theta} + g_2(r)e^{i3\theta}, \tag{4}$$

where $g_1(r)$ and $g_2(r)$ fall off like $1/r^2$ for $r \gg \xi_d \equiv \sqrt{\gamma_d/|\alpha_d|}$. Thus asymptotically the superconductor is not in a pure d-wave state, but rather in a state characterized by power law decay of the s-wave component. Only at the length scale given by the penetration depth is the pure d-wave state regained. Furthermore, close to T_d, $g_2(r) \approx -3g_1(r)$, and therefore the winding number far from the core is $+3$. This result combined with the result that close to the core the winding number is -1 [8] forces us to conclude that four additional positive vortices must exist in $s(r,\theta)$ outside the core. We emphasize that this is a topological result and thus not sensitive to small modifications of the parameters. As is shown below, these vortices lie on the $\pm x$ and $\pm y$ axes. At lower temperatures a topological transition to a state with s-wave winding number -1 is in principle possible.

We have studied the dependence of the maximum of the s-wave component on the GL parameters. Noting that both the d-wave and s-wave components rise over the same length scale given by ξ_d allows us to give an order of magnitude estimate for the magnitude of the s-wave order parameter at the maximum,

$$\max(s)/d_0 \sim \gamma_v/\alpha_s\xi_d^2. \tag{5}$$

Our numerical results confirm that the constant of proportionality is of order unity. Note that the temperature dependence of max(s) is $(1 - T/T_d)^{3/2}$.

In Fig. 1 we show the behavior of the s-wave amplitude along the x axis and along the diagonal, as obtained by numerical integration of Eqs. (2). Along the diagonals, s has peaks whose amplitude is given by Eq. (5). Along $\pm x$ and $\pm y$, s has nodes corresponding to the four positive vortices mentioned above. The region inside these nodes corresponds to the core region with the domain structure described in Ref. [2]. Outside these nodes, $s(r,\theta)$ is well described by Eq. (4).

Next we turn to the problem of the structure of the vortex lattice in the vicinity of the upper critical field H_{c2}, where the amplitudes of the order parameters are small and it is sufficient to consider the linearized GL equations. It is easily seen that in the Landau gauge ($\mathbf{A} = \hat{\mathbf{y}}Bx$) these linearized field equations are satisfied by taking $d(\mathbf{r}) = e^{iky}d(x)$, $s(\mathbf{r}) = e^{iky}s(x)$. Then, exactly as in the one component case [9], we are left with a one-dimensional problem which can be stated as follows:

$$
\begin{aligned}
(\mathcal{H}_0 + \alpha_d)d + Vs &= Ed, \\
Vd + (\mathcal{H}_0 + \alpha_s)s &= Es,
\end{aligned}
\tag{6}
$$

where $\mathcal{H}_0 = \hbar\omega_c(a^\dagger a + 1/2)$ and $V = \epsilon_v(\hbar\omega_c/2)(a^\dagger a^\dagger + aa)$ are expressed in terms of the usual raising and lowering operators, which can be written as $a = [(x - x_k)/l + l(\partial/\partial x)]/\sqrt{2}$. Here $l = \sqrt{\hbar c/e^*B}$ is the magnetic length, $x_k = kl^2$, and $\omega_c = (e^*B/mc)$. In writing Eqs. (6), we have assumed, for simplicity, that $m_d^* = m_s^* \equiv m$, i.e., that $\gamma_d = \gamma_s$, and we have set $\epsilon_v = \gamma_v/\gamma_s = m_s^*/m_v^*$. By including the right hand side of Eqs. (6) we are considering a slightly more general problem: $E = 0$ corresponds to the physical solution for $B = H_{c2}(T)$, and solutions for $E < 0$ will be useful later when we consider the stability of various vortex lattice structures.

In contrast to the one component case, the linearized equations (6) have no obvious exact solutions. This is due to the coupling term V whose origin traces back to the mixed gradient term in the free energy (1). In what follows we construct a simple variational solution, which is likely to capture all the essential physics of the problem. To this end we define $\mathcal{H}^{\pm} = \mathcal{H}_0 \pm V$ and $\varphi^{\pm} = d \pm s$, in terms of which we can write the set of equations (6) as

$$\begin{pmatrix} \mathcal{H}^{+} + T - T^{*} & -\Delta T/2 \\ -\Delta T/2 & \mathcal{H}^{-} + T - T^{*} \end{pmatrix} \begin{pmatrix} \varphi^{+} \\ \varphi^{-} \end{pmatrix} = E \begin{pmatrix} \varphi^{+} \\ \varphi^{-} \end{pmatrix},$$

where we have defined $T^{*} = (T_d + T_s)/2$ and $\Delta T = T_d - T_s$. A nice feature of this representation is that for $\Delta T = 0$ the equations for φ^{+} and φ^{-} decouple, each becoming a simple harmonic oscillator problem. Motivated by this fact, we consider a variational solution to the full problem in terms of normalized ground state harmonic oscillator wave functions,

$$\varphi_k^{\pm}(x) = (\sigma_{\pm}/l\sqrt{\pi})^{1/2} e^{-\sigma_{\pm}^2 (x - x_k)^2/2l^2}. \qquad (7)$$

The variational parameters σ_+ and σ_- are determined by minimizing $\langle E \rangle$. If $\sigma_+ = \sigma \cos\vartheta$ and $\sigma - = \sigma \sin\vartheta$, this leads to

$$\frac{\langle E \rangle}{\Delta T} = \frac{T - T^{*}}{\Delta T} + \frac{1}{4}\left(\frac{\hbar\omega_c}{\Delta T}\right)\left[(1 + \epsilon_v)x + (1 - \epsilon_v)\frac{1}{x}\right] - \frac{1}{2}\sqrt{\frac{2x}{1 + x^2}}, \qquad (8)$$

where $x = \tan\vartheta$. The full minimization is governed by the parameters ϵ_v and $\Lambda = \hbar\omega_c/\Delta T$. In the low field limit, $\Lambda \ll 1$, $\sigma_+ \approx \sigma_- \approx 1$, while in the high field limit, $\Lambda \gg 1$, $\sigma_{\pm} \approx [(1 \pm \epsilon_v)/(1 \mp \epsilon_v)]^{1/4}$. It follows that at least intermediate values of Λ are required for appreciable effects from s-d mixing to occur. Otherwise the s component effectively vanishes.

Solutions to Eq. (8) with $\langle E \rangle = 0$ give the dependence of the upper critical field H_{c2} on the temperature. Whenever a finite admixture of the s component is present, a characteristic upward curvature is found near the critical temperature in $H_{c2}(T)$ [3,5]. Such curvature has been observed experimentally in both La-Sr-Cu-O and Y-Ba-Cu-O compounds [10].

Next we construct a vortex lattice. Consider a periodic solution of the form

$$\chi_{d/s}(\mathbf{r}) = \sum_n c_n e^{inqy}[\varphi_n^{+}(x) \pm \varphi_n^{-}(x)], \qquad (9)$$

where $\varphi_k^{\pm}(x)$ are defined by (7) and $k = qn$ (n integer), which gives periodicity in y with period $L_y = 2\pi/q$. Solution (9) will also be periodic in x provided that the constants c_n satisfy the condition $c_{n+N} = c_n$ for some integer N. In what follows we consider only the case of $N = 2$ so that $c_{2n} = c_0$ and $c_{2n+1} = c_1$. The period in the x direction is $L_x = 2l^2 q$, and it also follows that $BL_x L_y = 2(hc/e^{*}) = 2\Phi_0$, i.e., there are two flux quanta per unit cell. The resulting lattice may be thought of as centered rectangular with two quanta per unit cell or, equivalently, as an oblique lattice with lattice vectors of equal length and one flux quantum per unit cell. The parameter q controls the shape of the vortex lattice, and it is customary to describe this shape by the ratio $R = L_x/L_y = (l^2/\pi)q^2$. $R = 1$ corresponds to the square, while $R = \sqrt{3}$ corresponds to the triangular vortex lattice. The restriction to centered rectangular lattices is made primarily for computational convenience. However, it is compatible with recent experiments on $YBa_2Cu_3O_7$ which show evidence for an oblique vortex lattice with nearly equal lattice constants [6].

At $B \approx H_{c2}(T)$ all solutions of the form (9) are degenerate. It is the fourth order terms in the free energy that lift this degeneracy below H_{c2} and determine the vortex lattice configuration. Minimizing the total free energy yields

$$F_{\min} = -\frac{\langle f_2 \rangle^2}{4\langle f_4 \rangle} \equiv -\frac{1}{4} E^2 \beta_A^{-1}, \qquad (10)$$

where $\langle \cdots \rangle$ means integration over the volume of the system, f_2 and f_4 stand for quadratic and quartic parts of the free energy density (1), respectively, and β_A is the generalization of the usual Abrikosov parameter [9].

We have studied the dependence of β_A on R in various regions of parameter space. For values of ϵ_v close to 0, $\beta_A(R)$ is minimized by $R_{\min} = \sqrt{3}$, i.e., the triangular lattice is stabilized. This is because, for ϵ_v small, the s component is suppressed and the usual one component solution [9,11] is found. As ϵ_v is increased, the minimum of β_A moves toward smaller values of $R_{\min} < \sqrt{3}$ and an oblique vortex lattice is preferred. Finally, at some value of ϵ_v (which depends on other parameters) the minimum of β_A reaches $R_{\min} = 1$, characteristic of the square vortex lattice. Further increase of ϵ_v has no effect on the lattice structure which remains square. The typical dependence of β_A on R is displayed in Fig. 2.

It follows that in a d-wave superconductor one should observe a general oblique vortex lattice, unless the material is in one of the limiting regimes where ϵ_v is very small or very large. Such an oblique lattice structure has,

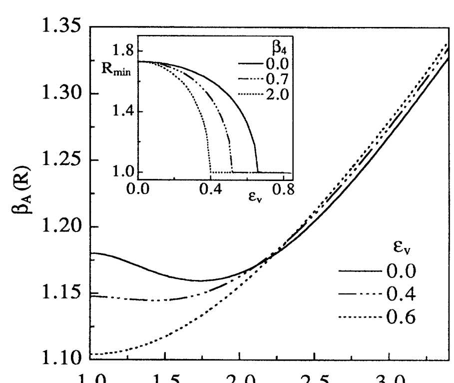
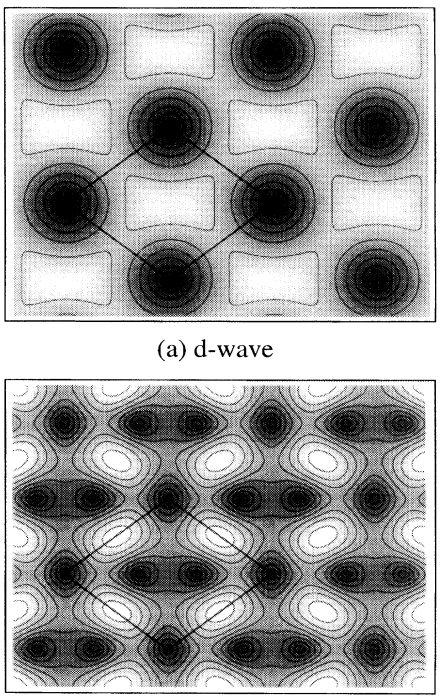


FIG. 2. Abrikosov ratio β_A as a function of the lattice geometry factor $R = L_x/L_y$ for different values of ϵ_v and $T_s = 0.5T_d$, $T = 0.75T_d$, $\beta_1 = \beta_2 = \beta_3 = \beta_4 = 1$, and $B = 0.8H_{c2}$. The inset shows the dependence of the minimum $R_{\min}$ on the parameter ϵ_v for different values of β_4.

in fact, been recently observed by SANS on $YBa_2Cu_3O_7$ single crystals in strong magnetic fields parallel to the c axis by Keimer *et al.* [6]. These authors reported an oblique lattice structure with nearly equal lattice constants and an angle of $\phi = 73°$ between primitive vectors. Our phenomenological theory is consistent with any angle ϕ in the interval $[60°, 90°]$, including that found experimentally. We display an example of a general oblique vortex lattice obtained by explicitly evaluating amplitudes of s and d components of the order parameter from Eqs. (9) in Fig. 3. A comparison of Figs. 3(a) and 3(b) reveals that the nontrivial nodal structure of the s component persists even in this high field regime.

Keimer *et al.* further report that one principal axis of the oblique unit cell is always found to coincide with the (110) or $(1\bar{1}0)$ directions of the $YBa_2Cu_3O_7$ crystal. This is at variance with our results, since we find that one lattice vector of the larger rectangular cell is oriented along (100) or (010), even in the presence of a small orthorhombic distortion. However, we find that the energy cost of rotating the vortex lattice is small compared to the energy needed to deform the lattice. It is thus possible that (110) twin boundaries, where the order parameter is weakened, bind lines of vortices and hence orient one of the oblique lattice vectors along (110) as is found experimentally.



(a) d-wave

(b) s-wave

FIG. 3. Contour plot of the amplitudes of (a) d component and (b) s component of the order parameter. GL parameters are the same as in Fig. 2 with $\epsilon_v = 0.45$, resulting in an oblique vortex lattice with $R_{\min} = 1.29$ and the angle between primitive vectors $\phi = 76°$. The lightest regions correspond to the largest amplitudes.

In closing, we note that the most striking feature of our calculations, the rich topological structure of the s-wave order parameter, might be observed experimentally by scanning Josephson tunneling from an s-wave tip into a truly tetragonal $d_{x^2-y^2}$ superconductor.

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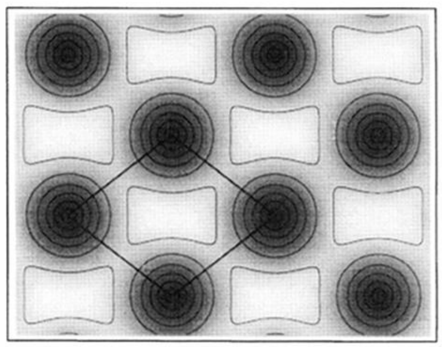
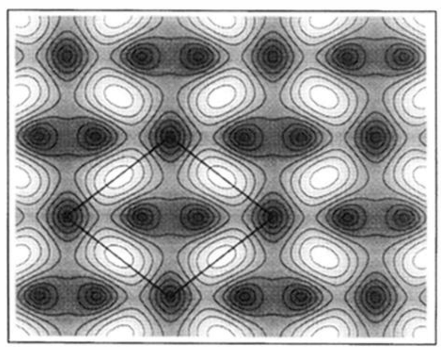


(a) d-wave



(b) s-wave

FIG. 3. Contour plot of the amplitudes of (a) d component and (b) s component of the order parameter. GL parameters are the same as in Fig. 2 with $\epsilon_v = 0.45$, resulting in an oblique vortex lattice with $R_{\min} = 1.29$ and the angle between primitive vectors $\phi = 76°$. The lightest regions correspond to the largest amplitudes.