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 $d_{2x-y^2}$ 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 counter-rotating unit vortex, centered by the core, surrounded by four symmetrically placed positive unit vortices. The Abrikosov lattice is shown to have a triangular structure close to $T_c$ and an oblique structure at lower temperatures. Comparison is made to recent neutron scattering data.

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Evidence continues to accumulate for the existence of nodes in the gap of high $T_c$ superconductors [1], although the nature of the microscopic mechanism remains controversial. Thus there is good reason to study the phenomenology of superconductors with non-trivial gap structures, particularly their behavior in an applied magnetic field that penetrates the superconductor, creating vortices which then play a dominant role in the transport properties of the system. 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, which was first derived by Joynt [3], served to interpret our results. The GL theory involves both the $d$-wave order parameter and an induced $s$-wave order parameter which arises through a mixed gradient coupling.

$$ f = \alpha_s |s|^2 + \alpha_d |d|^2 + \beta_1 |s|^4 + \beta_2 |d|^4 + \beta_3 |s|^2|d|^2 + \beta_4 (s^2 d^2 + d^2 s^2) + \gamma_s |\Pi|s|^2 + \gamma_d |\Pi|d|^2 + \gamma_v \left[ (\Pi^*_y s^*(\Pi^*_y d) - (\Pi^*_x s^*)(\Pi^*_x d) + c.c. \right]. $$ (1)

Here $\bar{\Pi} = -i\hbar \nabla - e^* A/c$, and $d$ is assumed to be the critical order parameter, i.e., we take $\alpha_s = T - T_s$, $\alpha_d = T - T_d$ with $T_s < T_d$. It is also assumed that $\beta_1, \beta_2, \beta_3, \gamma_s, \gamma_d$ and $\gamma_v$ are all positive [1]. The parameters $\gamma_i$ are related to the effective masses in the usual way. We use $\gamma_i = \hbar^2 / 2m_i^*$, for $i = s, d, v$. The field equations for the order parameters are obtained by varying the free energy (1) with respect to conjugate fields $d^*$ and $s^*$, giving,

$$ \left( \frac{\hbar^2}{2m_s} \Pi^{2} + \alpha_s \right) s + \frac{\hbar^2}{2m_v} (\Pi^*_y - \Pi^*_x) s + 2 \beta_1 |s|^2 s + 2 \beta_3 |s|^2 d s + 2 \beta_4 s^2 d^* = 0, $$ (2a)

$$ \left( \frac{\hbar^2}{2m_d} \Pi^{2} + \alpha_d \right) d + \frac{\hbar^2}{2m_v} (\Pi^*_y - \Pi^*_x) d + 2 \beta_2 |d|^2 d + 2 \beta_3 |s|^2 d + 2 \beta_4 s^2 d^* = 0. $$ (2b)

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 et al. [2] have previously shown that for a \( d \)-wave order parameter with the asymptotic form,
\[
d(r, \theta) = d_0 e^{i\theta},
\]
where \( d_0 = \sqrt{-\alpha_d/2\beta_2} \), the asymptotic form of the \( s \)-wave order parameter is:
\[
s(r, \theta) = g_1(r)e^{-i\theta} + g_2(r)e^{i3\theta},
\]
where \( g_1(r) \) and \( g_2(r) \) fall off like \( 1/r^2 \) for large \( r \). 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 \( -1 \), forces us to conclude that four additional positive vortices must exist 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.

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.

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 \( \xi_d \), where \( \xi_d^2 = \gamma_d/|\alpha_d| \), allows us to give an order of magnitude estimate for the magnitude of the \( s \)-wave order parameter at the maximum,
\[
\frac{\max(s)}{d_0} \sim \frac{\gamma_v}{\alpha_s \xi_d^2}.
\]

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

In Figure 4 we show the behavior of the \( s \)-wave amplitude along the \( x \)-axis and along the diagonal, as obtained by numerical integration of Eqs. 3. Moving outward from the center of the vortex both the \( s \)- and \( d \)-wave amplitudes increase over the same length scale \( \xi_d \). Moving further out one enters a region where the relative phase tends to lock to value \( \pm \pi/2 \). The change in the relative phase takes place in narrow “domain walls”. Up to this distance the results are in perfect agreement with the ones obtained within Bogoliubov-de Gennes theory [3]. However, further out the situation changes. The domains of rapid variation of the relative phase vanish. Furthermore, the relative phase starts to wind in the opposite direction. In Figure 8 this change manifests itself as a zero in the amplitude of the \( s \)-wave component. This zero is nothing but the core of one of four “extra” vortices. Identical vortices are found at all the four “wall ends”;

this combined with the vortex with an opposite charge at the center gives the total required winding of \( +3 \).

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 \((A = \dot{y}Bx)\) these linearized field equations are satisfied by taking \( \mathbf{d}(r) = e^{i\Phi_0}d(x), \quad \mathbf{s}(r) = e^{i\Phi_0}s(x) \). Then, exactly as in the one component case [3], we are left with a one dimensional problem which can be stated as follows:
\[
(\mathcal{H}_0 + \alpha_d)d + Vs = Ed, \quad (6a)
\]
\[
Vd + (\mathcal{H}_0 + \alpha_s)s = Es, \quad (6b)
\]
where \( \mathcal{H}_0 = \hbar \omega_c(a^\dagger a + 1/2) \) and \( V = \epsilon_v(\hbar \omega_c/2)(a^\dagger a + aa) \) 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 \( l = \sqrt{\hbar c/e^2B} \) is the magnetic length, \( x_k = kl^2 \) and \( \omega_c = (e^2B/mc) \). In writing Eqs. 6, we have assumed, for simplicity, that \( m^* = m^*_s = m \), i.e. that \( \gamma_d = \gamma_s \), and we have set \( \epsilon_v = \gamma_v/\gamma_s = m^*_s/m^* \). 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 Eqs. 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 [3]. 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 \( \mathcal{H} = \mathcal{H}_0 \pm V \), 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 \( T^* = (T_d + T_s)/2, \Delta T = T_d - T_s \). A nice feature of this representation is that for \( \Delta T = 0 \) the equations for \( \varphi^+ \) and \( \varphi^- \) 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,
\[
\varphi_k^\pm(x) = \sqrt{\frac{\sigma_k}{\sqrt{\pi}}} e^{-\sigma_k^2(x-x_k)^2}/2. \quad (7)
\]

The variational parameters \( \sigma_+ \) and \( \sigma_- \) will be determined by minimization of the eigenvalue \( \langle E \rangle \). If \( \sigma_+ = \sigma \cos \vartheta \) and \( \sigma_-= \sigma \sin \vartheta \), the resulting expression for \( \langle E \rangle \) can be minimized with respect to \( \sigma^2 \) analytically. This leads to
\[
\frac{\langle E \rangle}{\Delta T} = \frac{T - T^*}{\Delta T} + \frac{1}{4} \left( \frac{\hbar \omega_c}{\Delta T} \right) \left[ (1 + \epsilon_v)x + (1 - \epsilon_v) \frac{1}{x} \right] - \frac{1}{2} \sqrt{\frac{2x}{1 + x^2}}.
\]

where \( x = \tan \vartheta \). The last equation must be minimized numerically with respect to \( x \), and is governed by the parameter \( \Lambda = \hbar \omega_c / \Delta T \). In the low field limit, set by \( \Lambda \ll 1 \), \( \sigma_+ \approx \sigma_- \approx \sqrt{m \omega_c / \hbar} \), while in the high field limit, \( \Lambda \gg 1 \), \( \sigma_+ \approx \sigma_- \approx \sqrt{m \omega_c / \hbar} (1 + \epsilon_v)(1 + \epsilon_v) \). It follows that at least intermediate values of \( \Lambda \) 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 \( H_{c2}(T) \). Such curvature has been experimentally observed in both La-Sr-Cu-O and Y-Ba-Cu-O compounds \( \beta \), and has also been interpreted as a result of \( s-d \) mixing by Joynt \( \beta \).

We next construct a vortex lattice. Consider a periodic solution of the form

\[
\chi_{d/(s)}(r) = \sum_n c_n e^{iq_ny}[\varphi_n^+(x) \pm \varphi_n^-(x)],
\]

where \( \varphi_n^\pm(x) \) are defined by \( \beta \) and \( k = qn \), \((n \text{ integer)}\), which gives periodicity in \( y \) with period \( L_y = 2\pi / q \). Solution \( \beta \) 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 \( L_x = 2\pi q \), and it also follows that \( BL_x L_y = 2hc/\epsilon_s = 2\Phi_0 \), 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, \( R = L_x / L_y = ((2/\pi)q)^2 \). \( R = 1 \) 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\(_2\)Cu\(_3\)O\(_7\) which show evidence for an oblique vortex lattice with nearly equal lattice constants \( \beta \).

At \( B \approx H_{c2}(T) \) all solutions of the form \( \beta \) 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. Consider the solution to the full nonlinear problem of the form \( (s, d) = c(\chi_s, \chi_d) \) where \( c \) is an arbitrary constant. Then the total integrated free energy of the system becomes \( F = |c|^2 \langle f_2 [\chi_s, \chi_d] \rangle + |c|^4 \langle f_4 [\chi_s, \chi_d] \rangle \), where \( \langle \ldots \rangle \) means integration over the volume of the system, and \( f_2 \) and \( f_4 \) stand for quadratic and quartic parts of the free energy density \( \beta \) respectively. One can now minimize the total free energy \( F \) with respect to \( |c|^2 \) to obtain

\[
F_{\text{min}} = -\frac{(f_2)^2}{4(f_4)} \equiv -E^2 \beta_A^{-1},
\]

where \( \beta_A \) is the generalization of the usual Abrikosov parameter \( \beta \).

We have studied the dependence of \( \beta_A \) on \( R \) in various regions of the parameter space. The qualitative features of this dependence are most strongly influenced by the parameter \( \epsilon_v \). In particular, for values \( \epsilon_v \) close to 0, \( \beta_A(R) \) is minimized by \( R_{\text{min}} = \sqrt{3} \), i.e. the triangular lattice is stabilized. This is to be expected, since in this limit \( \sigma_+ \approx \sigma_- \), so the \( s \)-component is suppressed and the usual one component solution \( \beta \) is found. The consistency of our solution is confirmed in this limit where we recover the correct value of the Abrikosov ratio \( \beta_A(\sqrt{3}) = 1.1596 \) as quoted by Kleiner et al. \( \beta \). However as \( \epsilon_v \) is increased, the minimum of \( \beta_A \) moves toward smaller values of \( R_{\text{min}} < \sqrt{3} \) signaling that an oblique vortex lattice is preferred. Finally, at some value of \( \epsilon_v \) (which depends on other parameters) the minimum of \( \beta_A \) reaches \( R_{\text{min}} = 1 \), characteristic of the square vortex lattice. Further increase of \( \epsilon_v \) has no effect on the lattice structure which remains square. The typical dependence of \( \beta_A \) on \( R \) is displayed in Figure \( \beta \).

For all different parameter combinations studied, the minimum \( R_{\text{min}} \) varies continuously with \( \epsilon_v \). Varying other parameters changes somewhat the quantitative behavior of this dependence, but the essential qualitative features described above remain intact. For example, increasing the parameter \( \beta_A \) makes the transition from triangular to square lattice somewhat sharper (see inset of Figure \( \beta \)). One would also expect the inclusion of three dimensional screening effects (i.e. replacing \( B = H \) with \( B = H + \langle h_s \rangle \), where \( \langle h_s \rangle \) is calculated self-consistently) to change the results quantitatively, but not qualitatively.

In practice this continuous dependence would mean that in a \( d \)-wave superconductor one would expect to observe a general oblique vortex lattice, unless the material is in one of the limiting regimes where \( \epsilon_v \) is very small or very large. Such an oblique lattice structure has in fact been recently observed by SANS on YBa\(_2\)Cu\(_3\)O\(_7\) single crystals in strong magnetic fields parallel to the \( c \) axis by Keimer et al. \( \beta \). These authors reported an oblique lattice structure with nearly equal lattice constants and an angle of \( \phi = 73^\circ \) between primitive vectors. Our phenomenological theory is consistent with any angle \( \phi \) of the interval \( (60^\circ, 90^\circ) \), 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. \( \beta \) in Figure \( \beta \). Comparison of Figures \( \beta \) and \( \beta \) reveals that
the non-trivial topological 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 (1̅10) direction of the YBa$_2$Cu$_3$O$_7$ 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 note 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.

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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: $\gamma_s = \gamma_d = \gamma_v$, $\alpha_s = 10|\alpha_d|$, $\beta_s = \beta_d = 0$, and $\beta_s = 0.5\beta_d$. The inset shows schematically the positions of the s-wave vortices and their relative windings.

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

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 Figure 2 with $\epsilon_v = 0.45$, resulting in an oblique vortex lattice with $R_{\text{min}} = 1.25$ and the angle between primitive vectors $\phi = 76^\circ$. The lightest regions correspond to the largest amplitudes.