Vortex states in an unconventional superconductor and the mixed phases of UPt$_3$

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Recent experiments on UPt$_3$ indicate the existence of more than one superconducting phase and an associated unconventional order parameter belonging to a nontrivial representation of the crystal point group $D_{6h}$. In this article we consider the Ginzburg-Landau (GL) theory for the vortex states in the two-dimensional $E_1$ representation for the order parameter, the representation believed to describe the phases of UPt$_3$. One of the zero-field superconducting phases is predicted to break time-reversal symmetry. We show that the lower critical field for vortex nucleation in a ground state with broken time-reversal symmetry exhibits a novel asymmetry. Observation of this asymmetry in any superconductor would provide clear evidence for an unconventional order parameter. We present solutions to the GL equations for singly quantized vortices. For rectilinear vortices along the $c$ axis two classes of solutions are found: (i) axially symmetric vortices and (ii) nonaxisymmetric vortices which spontaneously break the axial symmetry of the condensate density. We discuss the structure of these vortices, their relation to the asymmetry of $H_{c1}$, the possibility of phase transitions between vortex states of different symmetry, and the phase diagram of UPt$_3$ in the $H$-$T$ plane.

I. INTRODUCTION

The heavy-fermion superconductors have stimulated considerable experimental and theoretical interest in part because they may exhibit unconventional pairing with an order parameter that breaks the point-group symmetry of the normal-metallic phase. This is particularly true for the heavy-fermion metal UPt$_3$, in which measurements of the low-temperature ultrasonic attenuation, specific heat, nuclear-spin relaxation, and thermal conductivity all show qualitatively different behavior from that predicted by the BCS theory for a conventional superconductor (for a recent review see Fisk et al.\textsuperscript{1}). The order parameter for an unconventional superconductor may have more degrees of freedom than the simple scalar amplitude that describes a conventional superconductor—leading to a number of novel properties and the possibility of more than one superconducting phase (for recent theoretical reviews see Rainer\textsuperscript{2} and Gor'kov\textsuperscript{3}). This paper is motivated in part by experimental measurements in the mixed states of UPt$_3$ where there appears to be more than one possible vortex phase,\textsuperscript{4–7} but much of this paper is applicable or easily generalized to other models of unconventional superconductivity.

Further evidence that UPt$_3$ is an unconventional superconductor comes from measurements on single crystals. The heat-capacity measurements of Fisher et al.\textsuperscript{8} show two anomalies (peaks) separated by $\sim 60$ mK (compared to $T_c \sim 0.5$ K), suggesting the presence of two nearly degenerate superconducting states. Anomalies in the ultrasonic attenuation in UPt$_3$ have also been reported. The $\lambda$ peak\textsuperscript{9} occurs $30-60$ mK below the superconducting transition as measured by ac susceptibility techniques. Similarly, the rf susceptibility measurements of Shivaram et al.\textsuperscript{10} show a peak roughly $30$ mK below the onset of superconductivity. All of these anomalies apparently occur in single crystals of UPt$_3$ with high purity (i.e., high transition temperatures), suggesting that the "splitting" of the transition is an intrinsic property of UPt$_3$. The appearance of two anomalies closely spaced in temperature is strong evidence for an unconventional order parameter in UPt$_3$ with a dimensionality greater than one.\textsuperscript{11–13} (The dimensionality of the order parameter is defined here to be that of the corresponding irreducible representation to which it belongs. Thus, any conventional order parameter, which belongs to the unit representation, is one dimensional.)

Longitudinal sound attenuation measurements in UPt$_3$ by Qian et al.\textsuperscript{4} and Müller et al.\textsuperscript{5} in a magnetic field oriented along or nearly along the $c$ axis show a peak at a relatively high-field strength, $H_{FL} \approx 1.2T \approx 0.6 H_{c1}$. This same anomaly has also been observed for other field orientations by Schenstrom et al.\textsuperscript{6} Torsional oscillator measurements of dissipation in the mixed state of UPt$_3$ by Kleiman et al.\textsuperscript{7} also show anomalies. The ultrasonic measurements prompted immediate speculation that the absorption peak signals a phase transition,\textsuperscript{4,5} with two obvious possibilities: (i) a structural transition of the flux lattice in which the symmetry of the flux lattice changes at $H_{FL}$ — the transition being driven by an anisotropic interaction between vortices, or (ii) a vortex-core transition analogous to that in $^3$He-B (Ref. 14) in which the symmetry and structure of the order-parameter change within the core of each vortex. Such a transition may also be accompanied by a change in the symmetry of the flux lattice. In either case, the existence of a transition for the field along an axis of sixfold symmetry suggests that the order parameter for UPt$_3$ has lower symmetry than that of the crystal and is multidimensional. Group-theoretical analysis,\textsuperscript{15} assuming strong spin-orbit coupling, shows that barring accidental degeneracy between two or more representations the highest dimen-
sional order parameter for UPt$_3$ is either of the 2D representations, $E_1$ or $E_2$. However, order parameters with dimensionality greater than two are possible for odd-parity states if spin-orbit coupling is ineffective.

This article is organized as follows: in Sec. II we summarize the symmetry classification of the superconducting states of UPt$_3$ and introduce the order parameter associated with the two-dimensional, even-parity, $E_{2g}$ (or odd-parity, $E_{1u}$ and $E_{2u}$) representations. We also discuss the Ginzburg-Landau (GL) free energy and review the results for the equilibrium phases in zero field. In Sec. III, we discuss the broken time-reversal symmetry of the equilibrium state in zero field and show that it leads to a novel asymmetry in the lower critical field. Observation of this asymmetry would clearly identify UPt$_3$ as a superconductor with an unconventional order parameter. Numerical solutions of the GL equations for a single vortex in the ground state with broken time-reversal symmetry are presented and discussed. The important features of these solutions are that: (1) three classes of vortex states, each with a single flux quantum, are stable depending on the values of the coefficients of the GL function, (2) in two of these classes the vortex solutions spontaneously break the $C_6$ symmetry of the equilibrium condensate density in the vicinity of the core (i.e., over roughly 10 coherence lengths), and (3) for these nonaxisymmetric vortices the order parameter in the vortex core is different than that of the ground state, whereas the vortex with axial symmetry is approximately the ground-state order parameter everywhere, but with reduced amplitude in the core. Section IV describes the vortex lattice and possibilities for phase transitions between vortex states of different symmetry and discusses recent theoretical work attempting to explain the observed transition in the mixed state of UPt$_3$.

II. UNCONVENTIONAL ORDER PARAMETERS, THE FREE ENERGY AND UP$_3$

Unlike conventional superconductors in which the order parameter has the symmetry as the underlying crystal lattice, an unconventional order parameter has lower symmetry. More precisely, an order parameter is unconventional if there exists a symmetry operation (other than a gauge transformation), $R \in G$, where $G$ is the symmetry group of the normal state, for which $R \Delta(R^{-1}k) \neq \Delta(k)$. The symmetry group of the order parameter is a subgroup of the full group $G$, and determines, for instance, the nodes in the energy gap for quasiparticle excitations, and therefore the thermodynamic and transport properties of the superconductor. Broken symmetries also give rise to new degrees of freedom, leading to additional collective modes of the order parameter and new dynamical phenomena peculiar to unconventional superconductors (cf. Ref. 16).

Superfluid $^3$He is the classic example of unconventional pairing in which rotational symmetries in spin and orbital spaces (as well as gauge symmetry) are broken (for a recent review see Fetter$^{17}$). The normal state of $^3$He is isotropic, but below $T_c$, $^3$He condenses into a superfluid state in which the Cooper pairs have angular momentum $l = 1$ and total spin $S = 1$. The basis functions describing these pairs are the $l = 1$ spherical harmonics, or equivalently the direction cosines $[\mathbf{x}, \mathbf{y}, \mathbf{z}]$ and the three symmetric Pauli matrices describing the spin triplet. The order parameter is then a tensor with nine complex amplitudes $A_{\alpha \nu}$, where $\alpha$ and $\nu$ refer to spin and orbital indices, respectively. Under the action of any element of the rotational symmetry group, $SO(3)_{spin} \times SO(3)_{orb}$, the order parameter transforms as $A_{\alpha \nu} = R_{\alpha \alpha'}A_{\alpha' \nu}R_{\nu \nu}'$, where $R$ and $R'$ represent rotations in spin and orbital space, respectively. Note that the order parameter does not transform into itself under the rotation group. The $A$ phase of $^3$He is described by the order parameter $\Delta \sim \bar{\mathbf{g}}(\mathbf{x} + i\mathbf{y})$ (up to any arbitrary rotation of the spin or orbital coordinates) corresponding to Cooper pairs with orbital angular momentum projection, $l_z = 1$ and equal amplitudes for $S_z = \pm 1$. Clearly the $A$-phase order parameter breaks time-reversal symmetry, as is indicated by the complex orbital part of the order parameter. Although unconventional superconductors differ significantly from superfluid $^3$He because the symmetry group is a discrete point group, an analogous order parameter to that in $^3$He appears to describe the superconducting state of UPt$_3$ [except close to $T_c$ (Ref. 12)].

The symmetry group of the normal state of UPt$_3$ is the hexagonal point group with twofold rotations about any of six symmetry axes in the plane perpendicular to the high-symmetry direction, combined with inversion, time-reversal and the gauge group; and is denoted by $G = D_{5h} \times T \times U(1)$. The superconducting classes, which define the possible symmetries of the superconducting ground state, are determined by the irreducible representations of $G$, and have been worked out by several authors$^{15,18}$ Since the normal state of UPt$_3$ has inversion symmetry, the equilibrium order parameter, at least near $T_c$ and barring the accidental degeneracy of two or more representations, will be either even or odd under inversion, in which case the order parameter is also either pure (pseudo)spin-singlet or (pseudo)spin-triplet. In either case there are four 1D ($A_1, A_2, B_1, B_2$) and two 2D ($E_1, E_2$) representations in the limit of strong spin-orbit coupling. These representations determine the dimensionality of the order parameter and the structure of the gap matrix, which are related as follows. The $2 \times 2$ gap matrix is resolved into its singlet and triplet parts,

$$
\Delta_{ag}(k) = \Delta_0(k) [i \sigma_y]_{ag} + \Delta(k) [i \sigma_y]_{ag} ,
$$

where

$$
\Delta_0(k) = \Delta_0(-k) \quad (\Delta(k) = - \Delta(-k))
$$

even the (odd) parity gap function. For the 2D representations,

$$
\Delta_0(k) = \eta_1 e_{\mu_1}^{i} (k) + \eta_2 e_{\mu_2}^{i} (k) ; \quad \mu = E_{1e}, E_{2g} ,
$$

in the even-parity case, and

$$
\Delta(k) = \eta_1 \sigma_1^{\mu_1} (k) + \eta_2 \sigma_2^{\mu_2} (k) ; \quad \mu = E_{1u}, E_{2u} ,
$$

for the odd-parity states. The basis functions $|e_{\mu}^i\rangle$ or $|\sigma^{\mu}_i\rangle$ transform as
The order parameter from microscopic considerations, rather we assume that the order parameter belongs to one of the two-dimensional representations already discussed. Almost all of the results that follow depend only on this assumption of two dimensionality for the order parameter, and are relatively insensitive to the particular 2D representation chosen \((E_{1g}, E_{1u}, E_{2g}, \text{or} \ E_{2u})\). Differences between the Ginzburg-Landau functionals and vortex solutions for the different 2D representations are discussed elsewhere.\(^{24}\) In the vicinity of \(T_c\), again barring the near degeneracy of two representations, the order parameter belongs to a single representation. The case of two nearly degenerate representations is considered in Refs. 25 and 26 for \(\text{UBe}_1\). The order parameter for any of the 2D representations \((E_{1g}, E_{1u}, E_{2g}, \text{or} \ E_{2u})\), is described by a pair of complex amplitudes, \((\eta_1, \eta_2)\). From either symmetry considerations\(^{15}\) or direct expansion of the BCS free-energy functional,\(^{24}\) the homogeneous free-energy functional (per unit volume) through sixth order in \(\eta_i\) is of the form,

\[
\frac{\Delta \Omega_{GL}[\eta_1, \eta_2]}{V} = \alpha(T)(|\eta_1|^2 + |\eta_2|^2) + \beta_1(1 + |\eta_1|^2 + |\eta_2|^2) + \beta_2|\eta_1|^2 + |\eta_2|^2 \nonumber \\
+ \gamma_1(|\eta_1|^2 + |\eta_2|^2)^2 + \gamma_2(|\eta_1|^2 + |\eta_2|^2)|\eta_1|^2 + |\eta_2|^2 \nonumber \\
+ \gamma_3(|\eta_1|^2 - |\eta_2|^2 - (9|\eta_1|^2|\eta_2|^2)^2(|\eta_1|^2 - |\eta_2|^2) - 3(\eta_1^* \eta_2^2 + \eta_2^* \eta_1^2)(|\eta_1|^2 - |\eta_2|^2) ,
\]

for any of the 2D representations. Since the vector representation is easier to describe, we cast our discussion in terms of this representation and simply remark that the results for the \(E_2\) representations may be obtained from those of the \(E_1\) by a straightforward mapping.\(^{24}\)

The equilibrium order parameter is determined by the minimum of the GL functional. Stability of all solutions to the minimization of the fourth-order functional requires that \(\beta_1 > 0\) and \(\beta_1 + \beta_2 > 0\). The sign of \(\beta_2\) determines the equilibrium phase: if \(\beta_2 > 0\) then the complex order parameter, \(\eta_+ = [-\alpha(T)/2B_1]^{1/2}(\hat{x} + i\hat{y})\), minimizes the free energy, and in zero field the time-reversed state, \(\eta_- = T\eta_+ = [-\alpha(T)/2B_1]^{1/2}(\hat{x} - i\hat{y})\) is degenerate with \(\eta_+\). However, for \(\beta_2 < 0\), the order parameter is real, of magnitude \(\eta = [-\alpha(T)/2(\beta_1 + \beta_2)]^{1/2}\), and is oriented in a direction determined by the sign of the sixth-order coefficient, \(\gamma_3\). For \(\gamma_3 > 0\) (\(\gamma_3 < 0\)), \(\eta = \bar{\eta} \hat{y}\) (\(\hat{x}\)) is stable. In either case, the six states obtained from rotations by multiples of \(\pi/3\) are degenerate. The time-reversal symmetry breaking phases, \(\eta_+\) and \(\eta_-\), are stable in weak-coupling BCS theory independent of the shape of the Fermi surface or the choice of basis functions.\(^{24}\)

The GL free-energy functional for spatially inhomogeneous states of the \(E_{1g}\) order parameter is constructed from the invariants of the 2D order parameter and the gradient operator.\(^{27}\) For the vector representation we obtain,

\[
\Delta \Omega_{GL}[\eta, \eta^*, A] = \int d^3x \left[ \alpha \eta \cdot \eta^* + \beta_1(\eta \cdot \eta^*)^2 + \beta_2|\eta|^2 \right] \nonumber \\
+ \int d^3x \left[ \kappa_1(D_i \eta_j)(D_j \eta_i)^* + \kappa_2(D_i \eta_j)(D_j \eta_i)^* + \kappa_3(D_i \eta_j)(D_j \eta_i)^* \right] \nonumber \\
+ \int d^3x \left[ \kappa_4(D_i \eta_j)(D_j \eta_i)^* + \int d^3x \left[ \frac{\partial \times A}{8\pi} - \frac{\mathbf{H} \cdot (\partial \times A)}{4\pi} \right] \right] ,
\]

where \(D_i = [\partial_i - i(2e/\hbar c)A_i] \) is the gauge-invariant derivative and \(A_i \) is the vector potential, and we have omitted the sixth-order terms. The order parameter in a magnetic field is determined by the Euler-Lagrange equations,

\[
\frac{\delta \Delta \Omega_{GL}[\eta, \eta^*, A]}{\delta \eta} = 0, \quad \frac{\delta \Delta \Omega_{GL}[\eta, \eta^*, A]}{\delta A_i} = 0 ,
\]

which give the GL differential equations,

\[
\kappa_1 D_i^2 \eta_j + \kappa_2 D_i \eta_j + \kappa_2 D_j \eta_i + \kappa_3 D_i^2 \eta_j - 2\beta_1(\eta \cdot \eta^*)\eta_i - 2\beta_2(\eta \cdot \eta)\eta_i^* = \alpha \eta_i ,
\]

\[
(\nabla \times \mathbf{h}) = - \frac{16\pi e}{\hbar c} \text{Im}[\kappa_1 \eta_j(D_i \eta_i)^* + \kappa_2 \eta_i(D_j \eta_j)^* + \kappa_3 \eta_j(D_j \eta_i)^* + \kappa_4 \delta_{ij} \eta_j(D_j \eta_i)^*] .
\]
The stiffness coefficients determining the gradient energies must be calculated from a more microscopic theory or obtained by comparison with experiment.

### III. \( H_{c2} \), VORTEX SOLUTIONS, AND BROKEN SYMMETRIES

The identification of unconventional superconductivity is difficult because there are but a limited number of unambiguous experimental tests of the broken symmetry exhibited by the order parameter; in addition, these experiments are often difficult to perform. Gor'kov\textsuperscript{29} has suggested a test for unconventional superconductivity in crystals with cubic or tetragonal point groups. In a conventional superconductor \( H_{c2} \) (in the GL limit) is independent of the direction of the field in the basal plane. Gor'kov, and later Burlachkov\textsuperscript{30} in greater detail, showed that the anisotropy of an unconventional order parameter would be exhibited by anisotropy of the slope of \( H_{c2} \) in the basal plane. A similar test of the broken symmetry of the point group was suggested by Joynt and Rice,\textsuperscript{30} who argued that an unconventional order parameter can induce a small but detectable strain in the crystal. More recently, Hirschfield\textsuperscript{31} proposed that for superconductors with a cubic point group, e.g., UBe\textsubscript{13}, the observation of a thermoelectric effect would be a definite signature of an unconventional order parameter.

We propose a test for unconventional superconductivity, applicable to any unconventional superconducting ground state with broken time-reversal symmetry.\textsuperscript{32} For an order parameter which breaks time-reversal symmetry, the lower critical field \( H_{c1} \) depends on whether the magnetic field is oriented parallel or antiparallel to the high-symmetry axis—more precisely in the case of the \( E_1 \) representation, the orientation of \( \mathbf{H} \) relative to the direction of the internal orbital momentum \( \text{Im}[\mathbf{\eta}^\ast \times \mathbf{\eta}] \), which itself is either parallel or antiparallel to the \( c \) axis for the states \( \mathbf{\eta}_+ \) or \( \mathbf{\eta}_- \), respectively.

The order parameter for conventional superconductors does not break time-reversal symmetry, since the action of time reversal on the order parameter can be removed by a trivial gauge transformation. An important feature of the zero-field order parameter obtained from weak-coupling theory for the vector representation is that it breaks time-reversal symmetry; the state \( \mathbf{\eta}_+ \) and its time-reversed partner \( \mathbf{\eta}_- \) are physically distinct, but degenerate in zero field. The degeneracy is lifted by a magnetic field, which leads to an asymmetry in the lower critical field, \( H_{c1} \) for flux entry into the superconductor. The lower critical field is determined by the self-energy of a vortex, or "line tension" (\( \epsilon_L = \text{energy per unit length of vortex} \)), \( H_{c1} = 4\pi \epsilon_L/\phi_0 \).

The physical distinction between the time-reversed states \( \mathbf{\eta}_+ \) and \( \mathbf{\eta}_- \) is that they represent Cooper pairs with opposite internal orbital angular momentum. This follows qualitatively from the Cooper pair amplitudes in the GL regime which are proportional to \( \Delta(k) \). Assuming the simplest form for the \( E_{1g} \) basis functions,

\[
\Delta_z(k) \sim k_z (k_x \pm i k_y) \sim Y_{2, \pm 1}(k)
\]

These degenerate order parameter states represent "d-wave" Cooper pairs with opposite angular momentum projections, \( l_z = \pm 1 \). For the case of \( E_{2g} \) the basis functions correspond to \( Y_{2, \pm 1}(k) \). Cooper pairs with a definite projection of internal orbital momentum will respond to the direction of the vortex supercurrent, \( \mathbf{v}_z \), which is determined by the magnetic field. We think of the vortex-core order parameter as a response to the circulating supercurrent. The energy of the vortex core generally depends on whether the internal motion of the pairs has the same or opposite circulation as the vortex supercurrent. Thus, the core energy for a vortex in the ground state \( \mathbf{\eta}_+ \) is different for a field \( \mathbf{H} \parallel \mathbf{2} (\mathbf{v}_z \sim \mathbf{\phi}) \) compared to \( \mathbf{H} \parallel -\mathbf{2} (\mathbf{v}_z \sim -\mathbf{\phi}) \). We calculate this energy difference (hereafter referred to as the energy "splitting") for vortices with \( \mathbf{v}_z \sim \mathbf{\phi} \) in the two time-reversed ground states \( \mathbf{\eta}_\pm \). This is equivalent to the energy splitting between vortices with opposite circulation in the fixed ground state, say \( \mathbf{\eta}_+ \). It is worth noting that preparation of a pure superconducting phase, i.e., without domains of the two degenerate phases \( \mathbf{\eta}_\pm \), is important for a clean detection of the field-reversal splitting of \( H_{c1} \). Note that if the zero-field ground state is prepared to be \( \mathbf{\eta}_+ \), application of a field below \( H_{c2} \) will not "flip" the state \( \mathbf{\eta}_+ \) into the state \( \mathbf{\eta}_- \) because there is no continuous symmetry connecting these states.

Near \( H_{c1} \) vortices are well separated relative to the size of the vortex core (\( \sim \) several \( \xi \)), so the mixed state at low fields may be described as an array of single vortices. We thus solve the GL equations for a single vortex in order to determine the core structure and current. The structure of the vortex lattice can then be obtained from the hydrodynamic interaction between neighboring vortices. For rectilinear vortices along the \( c \) axis the GL equations are independent of \( z \),

\[
|\alpha| \eta_1 - 2 \beta_1 \eta_1 (\eta_1 \eta_1^* - 2 \beta_2 \eta_2^* (\eta_1 \eta_1) \\
+ \kappa_1 D_j D_j \eta_1 + \kappa_2 D_j D_j \eta_1 + \kappa_3 D_j D_j \eta_j = 0 ,
\]

where repeated indices are summed over \( x \) and \( y \), and \( \alpha < 0 \) for \( T < T_c \). In addition one must satisfy the Maxwell equation,

\[
\frac{4\pi}{c} \textbf{j} = -(\hat{\alpha} \hat{\alpha} + \hat{\alpha} \hat{\alpha}^2) \textbf{A},
\]

with an appropriate choice of gauge. These equations are written in dimensionless form by scaling the order parameter components in units of the uniform equilibrium order parameter in zero field, \( \eta_0 = (|\alpha|/4\beta_1)^{1/2} \). The spatial coordinates are scaled in units of the GL coherence length,

\[
\xi = \left( \frac{\kappa_1 + \frac{1}{2} \kappa_2}{|\alpha|} \right)^{1/2},
\]

which, together with the penetration depth...
VORTEX STATES IN AN UNCONVENTIONAL . . .

\[ \lambda = \left( \frac{\phi_0^2}{64\pi^2 (\kappa_1 + \frac{1}{2}\kappa_3)^2 \eta_0^2} \right)^{1/2}, \quad (12) \]

are defined by considering the London limit of the GL equations. Finally, the vector potential is scaled in units of \( H_c \xi \), where \( H_c \) is the thermodynamic critical field.

\[ -\frac{1}{2\sqrt{2}\kappa_{GL}} \left[ (i\kappa_1 \tilde{\eta} \partial_i \eta_j + i\kappa_2 \tilde{\eta} \partial_i \eta_j + i\kappa_3 \tilde{\eta} \partial_i \eta_j) + (c. c.) \right] - \frac{1}{4\kappa_{GL}^2} \left[ 2\kappa_1 A_i \tilde{\eta} \eta_j + \kappa_2 A_j (\eta_i \eta_j + \eta_j \eta_i) \right] = -\partial_i A_i, \quad (14) \]

The scaled Maxwell-GL equations become

\[ \eta_i - \frac{1}{2} \eta_i (\eta_j \eta_j^* - \frac{1}{2} \beta \eta_j^* (\eta_j \eta_j^* + \kappa_1 D_j D_j \eta_j) \eta_j + \kappa_2 D_j D_j \eta_j + \kappa_3 D_j D_j \eta_j = 0, \quad (13) \]

and

\[ \left( \begin{array}{c} v_i \\ \bar{\rho}_i \end{array} \right) = \frac{\hbar}{2m} \left( \partial_i (x) + \frac{2e}{\hbar c} A_i \right), \quad (19) \]

are the superfluid velocity and superfluid density tensor. Since \( \bar{\rho}_i \) is diagonal and axially symmetric in the \( a-b \) plane, the superfluid velocity field is also axially symmetric far from the vortex core for vortices along the \( c \) axis. The phase is then, \( \partial x = \pm \phi \), where \( \phi \) is the azimuthal coordinate measured from the vortex core, the local boundary condition (in either ground state \( \eta_\pm \) is \( \eta(x) |_c = \eta_\pm e^{i\phi} \), where \( n \) is the winding number of the phase. It then follows that the vector potential far from the core has its London limit form.

We have solved the GL equations with these boundary conditions for a wide range of values of the scaled GL parameters \( \beta \) and \( \kappa \) and obtain two classes of vortex solutions for both ground states \( \eta_+ \) or \( \eta_- \). For \( \beta \geq 0.24 \), the solutions are analogous to those in conventional superconductors. The overall amplitude is axially symmetric and vanishes at the vortex center as shown in Fig. 1. The solutions are normalized to the equilibrium value \( \eta_0 \); we drop the tilde’s on \( \eta \) hereafter. This solution is favored for small values of \( \kappa \), especially for the ground state \( \eta_- \). Indeed for \( \kappa_2 = \kappa_3 = 0 \) the solution is everywhere proportional to the equilibrium order parameter,

\[ \eta_\pm(x) = f(r) \left[ \frac{\hat{z} + i\hat{y}}{\sqrt{2}} \right] \ e^{i\phi}, \quad (20) \]

where \( f(r) \) is the cylindrically symmetric solution for a conventional vortex. However, for smaller values of \( \beta \) and, to some extent, larger values of \( \kappa_2 \) the vortices exhibit broken rotational symmetry, as shown in Figs. 2 and 3 for the magnitude of the order parameter, \( |\eta(x)| \). Vortices in which the circulation is the same sign as the internal orbital momentum, e.g., \( \eta_+ e^{i\phi} \), have "triangular" cores (Fig. 2), whereas vortices with opposite circulation and internal orbital momentum, e.g., \( \eta_- e^{i\phi} \), have cores with a "crescent" shape (Fig. 3). In addition, for these vortices the magnitude of the order parameter does not vanish in the core. Conventional superconductors
FIG. 1. Axially symmetric vortex solution. The magnitude of $|\eta(x)|$ is shown for $\beta=0.3$ and $\kappa=0.1$; the core size is $\approx 2\xi$ and the order parameter vanishes at the center. The contour plot clearly shows the axial symmetry of $|\eta(x)|$.

respond to the diverging superfluid velocity of a vortex by forcing the order parameter to vanish at the singularity of the phase. For the 2D order parameter considered here, the boundary condition on the phase forces each amplitude to have its phase wind around the vortex core by $2n\pi$, and therefore, each amplitude must also vanish in order to eliminate the singularity in the phase. [There is no analog of the coreless vortices of $^3$He-A (Refs. 35 and 36) because there is no continuous rotational symmetry.] However, they need not do so at the same point, and in fact the vortices with nonzero amplitude in the core accomplish this by spatially separating the zeroes of the two amplitudes, as shown in Fig. 4. The order parameter in the region between the zeroes of $\eta_+^+$ and $\eta_+$ is different from the ground-state order parameter, and is in fact the time-reversed order parameter. This can be seen by projecting the order parameter $\eta(x)$ onto the basis

$${\eta}_+= (\hat{x}+i\hat{y})/\sqrt{2};$$

$$\eta = {\eta}_+(x)(\hat{x}+i\hat{y})/\sqrt{2}+{\eta}_-(x)(\hat{x}-i\hat{y})/\sqrt{2}.$$  

In Fig. 5(a) we show the amplitude $\eta_-$ of the time-reversed state for the vortex with $\eta(x)\to {\eta}_+e^{i\phi}$, i.e., the vortex of Fig. 2. Note that the phase of $\eta_-(x)$ [Fig. 5(c)] inside the core is essentially constant, i.e., there is no phase winding in the core. It is also interesting that the core amplitude also has zeroes; in fact $\eta_-$ has three zeroes [Fig. 5(a)], each corresponding to a phase winding of $2\pi$ for $\eta_-(x)$. This indicates that the triangular vortices have a residual $C_3$ symmetry. In particular the current has this symmetry. This contrasts with the dipolar splitting exhibited by the $\eta_+$ and $\eta_+$ components. The apparent contradiction with the $C_3$ symmetry of the $\eta_+$

FIG. 2. Nonaxially symmetric vortex for $\eta \sim (\hat{x}+i\hat{y})e^{i\phi}$. The upper figure shows $|\eta(x)|$ with a core size of $\approx 8\xi$ for $\beta=0.1$ and $\kappa=1.0$. The contour plot exhibits the residual $C_3$ symmetry of this nonaxially symmetric vortex. Note that $|\eta(0)| \approx 0.83$.  

FIG. 4. Axially symmetric vortex solution. The magnitude of $|\eta(x)|$ is shown for $\beta=0.3$ and $\kappa=0.1$; the core size is $\approx 2\xi$ and the order parameter vanishes at the center. The contour plot clearly shows the axial symmetry of $|\eta(x)|$.  

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component is resolved by examining the relative phase of \( \eta_+ \) and \( \eta_- \), which have different winding numbers. The dipolar splitting of \( |\eta_+| \) and \( |\eta_-| \) is obtained by constructing \( \eta_+ = \eta_+ + \eta_- \) and \( \eta_- = \eta_+ - \eta_- \) with the phase factors shown in Figs. 5(c) and 5(d). Vortices exhibiting spontaneously broken axial symmetry were first obtained by Thuneberg\(^{17}\) for \(^3\)He-B and also by Salomaa and Volovik.\(^{18}\) Many of the features of vortices in the superfluid \(^3\)He are exhibited by the vortex states of this 2D vector order parameter. For detailed discussions of the vortex states in superfluid \(^3\)He see the reviews by Fetter,\(^{17}\) Thuneberg,\(^{33}\) and Salomaa and Volovik.\(^{39}\)

We summarize these calculations in Fig. 6, showing the regions in the GL parameter space where these two classes of vortex solutions are found to be energetically stable. The boundary line separates vortex solutions with nonaxial cores (separated cores) from axial solutions (coincident cores). Axial vortices are obtained for relatively large values of \( \beta \), which determines the difference in condensation energy between different possible ground states. If \( \beta \gg 1 \) it costs a great deal of condensation energy to deform the vortex core into a state with symmetry different than the ground state, so the axially symmetric solution has lower energy. However, if the stiffness ratio is large enough it can pay to separate the two cores and lower the gradient energy at least for the crescent vortices.

The energies of these vortex solutions are calculated from the scaled GL free-energy functional,

\[
f = f_0 \mathbf{f} = -f_0 [e_i e_i^* - \frac{1}{4} (e_i e_i^*)^2 - \beta/4 |\eta_i| |\eta_j| - \mathbf{k}_i (D_i \eta_j)(D_j \eta_i)^* - \mathbf{k}_j (D_j \eta_i)(D_i \eta_j)^* - \mathbf{k}_3 (D_i \eta_j)(D_j \eta_i)^*]
\]

where \( f_0 = \frac{1}{4} |\alpha| |\eta_0|^2 \) is the free energy density of the homogeneous ground state. The total energy of the vortex state is calculated from the order-parameter configuration defined on the discrete lattice,

\[
\delta F = f_0 \mathbf{f}^2 \sum_{m,n} \mathbf{f}_m \mathbf{f}_n h^2,
\]

where \((m,n)\) label a lattice site and the discrete cell dimension is \( h \) (in units of a coherence length \( \xi \)).

The line tension of a vortex is the excess energy of the vortex state compared to the energy of the ground state in the absence of a vortex. This energy includes both the kinetic energy of the superconducting electrons and magnetic-field energy induced by the vortex current. However, in the limit \( \lambda/\xi \gg 1 \) the magnetic-field energy is small compared to the kinetic energy by a factor of \( 1/\ln(\lambda/\xi) \), which explains the lack of sensitivity of the solutions to the values of \( \kappa_{GL} \) and \( \kappa_2 - \kappa_3 \). The line tension is then,

\[
\epsilon_L = f_0 \mathbf{f}^2 \sum_{m,n} h^2 (f_m + 1) = f_0 \mathbf{f}^2 \varepsilon_L,
\]
where $\varepsilon_L$ represents the excess energy (in units of $f_0^2$) of the vortex, and is the quantity that determines the splitting of $H_{c1}$. As already discussed, the line tension for the vortices $\eta_+ e^{i\phi}$ and $\eta_+ e^{-i\phi}$ is different. In Fig. 7 we show the splitting,

$$\delta \equiv \frac{2(H_{c1}^+ - H_{c1}^-)}{(H_{c1}^+ + H_{c1}^-)}$$

(24)

as a function of $(\kappa_2 - \kappa_3)$ for $\beta = 0.1$. The splitting is a sizeable fraction of $H_{c1}$ except for $\kappa_2 - \kappa_3 \approx 0$, which is the weak-coupling prediction in the absence of impurity scattering. In principle $\kappa_2$ and $\kappa_3$ can be obtained from measurements of the upper critical field slopes at $T_c$ for several orientations of the field. However, from existing data on $H_{c2}$ we are unable to obtain $(\kappa_2 - \kappa_3)/\kappa_1$. Thus a precise prediction for the magnitude of the splitting is not currently possible; however, Choi and Muzikar\textsuperscript{40} show that non-s-wave impurity scattering leads to $\kappa_2 - \kappa_3 \approx \kappa_1(1/T_c)$. Strong-coupling corrections can also give sizeable values for $\kappa_2 - \kappa_3$. The linear dependence of $\delta$ on $(\kappa_2 - \kappa_3)$ can be obtained analytically from a variational form for the vortices,

$$\eta_\pm = \eta_0 f(r) e^{i\phi} \left( \hat{n} \pm i\hat{y} \right) \sqrt{2}$$

(25)

with $f \to 1$ as $r \to \infty$ in which case the free energy becomes,

$$\varepsilon_L = f_0 \int d^2x \left[ (f^2 - 1)^2 + \frac{2}{2} \left( \frac{f^2}{r^2} + f'^2 \right) \right]$$

$$+ 2(\kappa_2 - \kappa_3) \frac{f f'}{r}$$

(26)
provide an unambiguous identification of broken time-reversal symmetry of the superconducting order parameter.

IV. SYMMETRY OF THE VORTEX LATTICE

The Abrikosov lattice for a conventional isotropic superconductor with $\lambda \gg \xi$ is hexagonal. A hexagonal lattice is favored for extreme type-II conventional superconductors provided the crystal has at least fourfold rotational symmetry around the axis defined by the magnetic field. However, for an unconventional superconductor this is not generally the case because the superfluid density may be anisotropic even if the crystal has axial symmetry about the field. In addition the symmetry of the vortex lattice need not be the same for all fields and temperature regimes. In the low-field region, $H = H_{c1}$, the vortex lattice structure is determined by nearest-neighbor interactions between vortices, which for fields along the $c$ axis is
\begin{equation}
U(r_1-r_2) \propto K_0 \left\{ \left( x_1-x_2 \right)^2 / \lambda_\perp^2 + \left( y_1-y_2 \right)^2 / \lambda_\parallel^2 \right\}^{1/2},
\end{equation}
where $K_0(x)$ is the modified Bessel function and $\lambda_\perp$ and $\lambda_\parallel$ are the field penetration lengths perpendicular to the $c$ axis. Since these penetration lengths are determined by $\rho_s$ (1/$(\lambda_\perp^2 \lesssim \rho_s^x$, $1/\lambda_\parallel^2 \lesssim \rho_s^y$) the interaction between vortices is cylindrically symmetric provided $\rho_s^x=\rho_s^y$, in which case the vortex lattice is hexagonal. This is the case for the low-field flux lattice (where the distance between vortices is large compared with the core size, $d \gg \xi$) in either of the ground states $\eta_\pm \sim (\hat{x} \pm i \hat{y})$, even though the vortex cores break the axial symmetry of $\vec{p}_s$. Figure 8(a) shows triangular core vortices on a hexagonal lattice. In this low-field region there is a weak anisotropic interaction between vortices induced by the anisotropic vortex cores. The short-range anisotropy of the supercurrent that determines the anisotropy of the interaction is shown in Fig. 8(b).

The “triangular” core vortices break rotational symmetry, so the weak anisotropic interaction between these vortices may lead to orientational ordering at low fields. However, this orientational order cannot exist on a hexagonal lattice without frustration [Fig. 8(c)]. Further work is required to elucidate the symmetry and structure of the flux lattice for vortices with a long-range isotropic interaction and a short- or intermediate-range anisotropic interaction.

If the zero-field ground state is either of the real phases $\eta \sim \hat{x}$ or $\hat{y}$, which is expected to be the case very near $T_c$ in UPt$_3$,\cite{12} then the superfluid density tensor is anisotropic in the $x$-$y$ plane, i.e.,
\begin{equation}
\vec{\rho}_s \sim \begin{bmatrix}
\kappa_{123} & 0 & 0 \\
0 & \kappa_1 & 0 \\
0 & 0 & \kappa_4
\end{bmatrix}, \quad \eta \sim (1,0),
\end{equation}
and similarly with $\rho_s^{xx}, \rho_s^{yy}$ interchanged if $\eta \sim \hat{y}$. Since the superfluid density tensor is diagonal a scaling of the coor-
FIG. 8. Triangular vortices on a lattice. (a) At low fields $H \sim H_{c1}$ the lattice spacing is large compared with the vortex core, the vortex-vortex interaction is cylindrically symmetric, and the favored lattice is hexagonal. The vortex cores may order at low field. The short-range ($d \sim 10\xi$) anisotropic current density (b) generates a short-range anisotropic interaction between vortices which favors triangular vortices aligning their edges (c). On a hexagonal lattice the anisotropic interaction cannot be minimized for every pair of vortices. This "bond frustration" may be removed for triangular vortices on a honeycomb lattice (d).

FIG. 9. The GL phase diagram for solutions at $H_{c2}$ and $H||\hat{e}$ from Ref. 41. The line $\kappa_\perp = \kappa_1 + \kappa_2$ separates solutions corresponding to a hexagonal flux lattice (phase 0) and a nonhexagonal lattice (phase 2) [$H_2(x)$ is the second-order Hermite polynomial].

For intermediate fields, $H_{c1} \ll H < H_{c2}$, there are as yet no published theoretical calculations of the vortex lattice structure. However, the low- and high-field solutions for $H||\hat{e}$ suggest several interesting possibilities. For the nonaxisymmetric triangular vortices at intermediate distances, $d \sim 10-20\xi$, the vortex-vortex interaction is anisotropic and favors the alignment of vortices with their "edges" parallel [see Fig. 8(c)]. But, triangles cannot be placed on a hexagonal lattice without violating this "edge rule," thus leading to orientational frustration. There are then two possibilities for a purely structural vortex-lattice transition at intermediate fields. If the vortex cores are rigid at these fields and the line tension of the "triangular" vortices is much lower than the axially symmetric vortices, the favored lattice will be a honeycomb [Fig. 8(d)], which allows the edge rule to be satisfied, but reduces the number of nearest neighbors. The second possibility, favored if the difference in line energies between the triangular and axial vortices is relatively small compared to the anisotropic interaction energy between
triangular vortices is that the lattice remains hexagonal, but one third of the vortices have axially symmetric cores. A hexagonal lattice with six triangular vortices, all satisfying the edge constraint, and a single axial vortex in the center eliminates the orientational frustration. In either case a structural transition of the vortex lattice will occur when the vortex lattice spacing \( d \) is approximately equal to the core size, \( R_{\text{core}} \). In addition, as already mentioned, it is also possible that an orientational ordering transition occurs at a much lower field (larger lattice spacing) where the anisotropic vortex cores align relative to one another on a hexagonal lattice.

A vortex lattice transition at intermediate fields involving strictly rigid vortex cores is unlikely unless the difference in energy density between different vortex-core structures is relatively large compared to the vortex kinetic energy density in the vicinity of the core, and this will not be the case unless the stiffness coefficients controlling the kinetic energy are small compared to those controlling changes in the magnitude of the order parameter. The more likely case is that the order parameter in the region of the core of the nonaxisymmetric cores will deform as the vortex density rises and the interaction energy between neighboring vortices becomes an appreciable fraction of the vortex core energy. In this case a vortex-core transition between non-axial and axial vortices is possible, and the lattice spacing at which such a transition would occur we again expect to be \( d \sim R_{\text{core}} \), corresponding to a field

\[
H \approx H_{c2} \frac{8\pi}{\sqrt{3}} \left( \frac{\xi}{R_{\text{core}}} \right)^{2} \frac{\kappa_1}{\kappa_1 + 1/2\kappa_{23}}.
\]

Assuming the phase transition in UPt$_3$ at \( H_{FL} \approx 0.6H_{c2} \) is a vortex-core transition, we estimate the vortex-core size to be \( R_{\text{core}} = 5\xi \), a reasonable estimate for the nonaxisymmetric vortices. Although it is plausible that a transition involving nonaxisymmetric vortices occurs as a result of short-range \( (d \sim 6-10\xi) \) anisotropic vortex-vortex interactions, solutions to the GL equations in the intermediate-field region \( H_{c1} \ll H \ll H_{c2} \), are needed in order to test these speculations. Volovik has proposed that the high-field attenuation peak in UPt$_3$ (for \( H \approx 0 \)) represents a phase transition from a nonhexagonal flux lattice at low fields to a hexagonal lattice at high fields. He assumes that the ground state is one of the real order parameters, \( \eta \sim \tilde{x} \) or \( \tilde{y} \), and that the high-field \( (H \sim H_{c2}) \) phase is the solution of the linearized GL equations with \( \eta \sim \tilde{x} + i\tilde{y} \). Since the \( \eta \sim \tilde{x} \) ground state has an anisotropic superfluid density tensor in the \( x-y \) plane, the flux lattice

\[
\text{FIG. 10. Experimental phase diagram taken from Schenstrom et al. (Ref. 6). The } (H,T) \text{ values for the peak in the ultrasound attenuation are shown for several angles of the magnetic field relative to the } c \text{ axis: } \square(\theta_H = 0), \triangle(\theta_H = 45^\circ), \text{ and } \odot(\theta_H = 85^\circ), \text{ while the filled symbols denote the } \lambda \text{ peak for the corresponding orientations at low fields. The extrapolations suggest that the two phase boundaries represent different transitions.}
\]

\[
\text{FIG. 11. Phase diagram constructed from ultrasound data (Ref. 6), specific-heat data (Ref. 44), torsional oscillator measurements (Ref. 7), and upper critical-field measurements (Ref. 45). In zero-field, heat-capacity measurements show two transitions at } T_r \text{ and } T_{s*}. \text{ We label these Meissner states by the order parameters of } E_1 \text{ in Ref. 12. The } \lambda \text{ peak occurs at roughly the position of } T_{s*} \text{ in } H = 0. \text{ In low fields the } \lambda \text{ peak moves to slightly lower temperatures, and may intersect } H_{c2}(T). \text{ Based on the order parameter identifications shown, the phases II and III near } H_{c1} \text{ correspond to hexagonal } (T < T_{s*}) \text{ and nonhexagonal flux lattices. The symmetry of flux phase I is uncertain. The high-field attenuation peak } H_{FL}(T) \text{ separates two different flux phases and appears to intersect } H_{c2}(T) \text{ at finite field. Torsional oscillator measurements indicate a second phase line } H_{TO} \text{ at lower fields. The shaded region near } H_{c2}(T) \text{ where several phase lines extrapolate is unclear. Joyst suggests the } \lambda \text{ line and } H_{FL} \text{ should be identified as shown in the inset.}
\]
will be nonhexagonal; however, the $\hat{x} + i\hat{y}$ state supports a hexagonal vortex lattice. Thus, Volovik argues a transition should occur at some intermediate field. The arguments against this explanation are that the state $\eta \sim \hat{x}$ is not likely to be the ground state except very close to $T_c$. In fact the recent double transition observed in the heat-capacity measurements of Fisher et al. supports the identification of the zero-field order parameter as one of the doubly degenerate states $\eta_+ \sim (\hat{x} + i\hat{y})$, except in the narrow temperature range $\Delta T_c \sim 60$ mK of the first superconducting transition.  

Volovik also argues that this transition should not be present for $H_{||}\hat{c}$; however Schenstrom et al. observed the transition for all orientations of the magnetic field.

Joynt has proposed a similar explanation to that of Volovik. For zero-field he assumes the hexagonal symmetry of the crystal lattice is reduced by the antiferromagnetic ordering at $T_N \approx 5$ K, and that this reduction in symmetry leads to a splitting of the superconducting transition in zero field with $\eta \sim$ (Joynt’s “C-phase”) appearing at $T_c$, followed by $\eta \sim (\hat{x} \pm i\hat{y})$ (Joynt’s “A phase”), at a slightly lower temperature.  

Joynt identifies the $\lambda$ peak in zero field with the second transition. Joynt also argues that near $H_{c2}$ the order parameter is not the $n = 0$ solution with $\eta \propto (\hat{x} + i\hat{y})$ corresponding to a hexagonal flux lattice, but rather a state of the form, $\eta \sim (\hat{x} + ri\hat{y})\phi_0$, with real $r = \text{constant} < 1$ (Joynt’s “B phase”). He identifies $H_{c2}$ as the transition between these two states, which correspond to a hexagonal flux lattice at low fields and a nonhexagonal lattice at high fields. Although Joynt’s $B$ phase is not a solution of the GL equations (except for $r = 1$), Sundaram and Joynt have also obtained Zhitomirskii’s solution, which they argue is related to Joynt’s $B$ phase variational order parameter. Joynt’s interpretation identifies the transition line $H_{c2}$ with the $\lambda$ transition in zero-field (see the inset of Fig. 11) and requires the $C$ phase to deform continuously into the $B$ phase above the line $H_{c2}(T)$; the experimental data appear to conflict with this phase diagram. Extrapolations of the $\lambda$ peak measured by Schenstrom et al. for low fields, and the high-field peak do not join smoothly (see Fig. 10). The data indicate at least three flux phases and two Meissner phases as shown in Fig. 11. However, the phase diagram is not well characterized near $H_{c2}(T)$ and further experiments are needed in order to clarify the number of superconducting phases and the symmetry of the order parameters.

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FIG. 1. Axially symmetric vortex solution. The magnitude of $|\eta(x)|$ is shown for $\beta=0.3$ and $\bar{s}=0.1$; the core size is $\approx 2\xi$ and the order parameter vanishes at the center. The contour plot clearly shows the axial symmetry of $|\eta(x)|$. 
FIG 2. Nonaxially symmetric vortex for \( \eta = (\hat{x} + i\hat{y}) e^{-\beta} \). The upper figure shows \( |\eta(x)| \) with a core size of \( \approx 8\xi \) for \( \beta = 0.1 \) and \( \bar{r} = 1.0 \). The contour plot exhibits the residual \( C_1 \) symmetry of this nonaxially symmetric vortex. Note that \( |\eta(0)| = 0.83 \).
FIG. 4. Splitting of the vortex core. The plots of $|\eta_z(x,y)|$ and $|\eta_y(x,y)|$ for the triangular vortex of Fig. 2 show the separation of the zeroes for the two-order parameter components. Axially symmetric vortices correspond to the coincidence of these two nodes.
FIG. 6. Vortex phase diagram. Nonaxisymmetric triangular [crescent] vortices are stable for small positive $\beta$, to the left of the dark [light] boundary line for vortices with equal [opposite] signs for the internal orbital momentum and circulation, i.e., $\eta \sim (\hat{x} + i \hat{y}) e^{i\theta}[e^{-i\delta}]$. 
FIG. 8. Triangular vortices on a lattice. (a) At low fields \( H \sim H_{c1} \) the lattice spacing is large compared with the vortex core, the vortex-vortex interaction is cylindrically symmetric, and the favored lattice is hexagonal. The vortex cores may order at low field. The short-range \( (d \sim 10\xi) \) anisotropic current density (b) generates a short-range anisotropic interaction between vortices which favors triangular vortices aligning their edges (c). On a hexagonal lattice the anisotropic interaction cannot be minimized for every pair of vortices. This "bond frustration" may be removed for triangular vortices on a honeycomb lattice (d).