Properties of the flux-line lattice in anisotropic superconductors near H_{c2}

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Using anisotropic Ginzburg-Landau (GL) equations based upon a tensor effective-mass approximation, we study the vortex lattice geometry near the upper critical field H_{c2}. We employ a scaling technique to reduce the first GL equation to isotropic form. This permits simple evaluation of the angular dependence of the upper critical field for arbitrary mass anisotropy. Although the mass tensor cannot be scaled out of the second GL equation, the two equations may be solved and the free energy evaluated. In the high-κ limit appropriate, e.g., to the new high-temperature superconductors, the geometry of the fluxoid lattice is found to be hexagonal in scaled coordinates but with a preferred orientation relative to the underlying crystallographic axes. The internal magnetic fields both parallel and perpendicular to the vortex axis are determined for the special case of uniaxial anisotropy.

I. INTRODUCTION

The recent discovery of new high-temperature superconductors (HTSC's) has rekindled interest in the magnetic behavior of anisotropic type-II superconductors. Most HTSC's are highly anisotropic in both their normal and superconducting states due, e.g., to preferential current conduction in planar CuO arrays as in $YBa_2Cu_3O_7$. The symmetry of this latter compound is orthorhombic, but nearly tetragonal (uniaxial), while others like the Tl-based compounds are perfectly tetragonal.

In this work we consider the general problem of finding the equilibrium vortex lattice geometry in an anisotropic superconductor, for the case that the externally applied magnetic-field points in an arbitrary direction relative to crystallographic axes. This problem has recently been treated using a London approximation[1,2] appropriate for fields well below H_{c2}, and it was earlier investigated near H_{c2} using an anisotropic Ginzburg-Landau theory.[3,4] We also study the region near H_{c2}, and generalize the treatment of Ref. 3 to a mass tensor of arbitrary orthorhombic symmetry, such as is characteristic of most of the new HTSC's. Uniaxial symmetry is treated as a special case to make contact with earlier work, and as a useful first approximation for them.

Our paper is organized as follows. In Sec. II we write down the two Ginzburg-Landau (GL) equations using a mass tensor to describe the anisotropy. We then introduce a canonical but nonorthogonal scaling transformation applied to coordinates, momentum operators, the vector potential and the magnetic field, which has the effect of reducing the first GL equation to isotropic form. The transformed or scaled coordinates are shown to be related to the nonorthogonal coordinates employed by Kogan and Clem.[3]

Our transformation enables us to immediately apply to anisotropic superconductors any result for isotropic superconductors which depends only upon the *first* GL equation. As an example of this we derive the angular dependence of the upper critical field for an orthorhombic superconductor. Our result reduces to the well-known uniaxial angular dependence in the appropriate limit.[5]

While our transformation cannot eliminate the mass tensor from the second GL equation, we show how that equation too can be written in scaled form analogous to the isotropic case. A simple physical picture of the scaling is introduced to clarify its consequences.

In Sec. III we solve the GL equations by techniques similar to those used in isotropic formalism. In scaled space we define the zero-order solution for the order parameter, find its normalization condition, and calculate the free energy. For reasonably large κ the minimum-energy solution in scaled space is shown to be a regular equilateral triangular lattice, but with a preferred orientation to the underlying crystallographic axes. This orientation is shown to correspond to that of Campbell *et al.*,[1] derived in the London limit. The profiles of internal magnetic fields, both parallel and perpendicular to the fluxoid axis are also calculated. The latter depend upon the mass anisotropy and external field orientation, but are shown to reduce to a particularly simple form in the limit of very large anisotropy. The bulk magnetization is also computed and found to obey a generalized scaling relation first noted by Kogan and Clem.[3]

In Sec. IV we summarize our results in terms of the correspondences to and differences from isotropic superconductors.

II. THE SCALING TRANSFORMATION

The dominant features of highly anisotropic superconductors may be represented through the Ginzburg-Landau equations with a phenomenological tensor mass $\overline{\overline{M}}$ or its inverse.

$$\tfrac{1}{2}(-i\hbar\nabla - q\,\mathbf{A}/c)\cdot\overline{\overline{M}}^{-1}\cdot(-i\hbar\nabla - q\,\mathbf{A}/c)\psi + \alpha\psi + \beta|\psi|^2\psi = 0\ , \qquad (1)$$

$$\nabla\times\mathbf{H}=4\pi\mathbf{J}/c$$
$$=(2\pi q/c)\overline{\overline{M}}^{-1}\cdot[\psi^*(-i\hbar\nabla-q\,\mathbf{A}/c)\psi+\text{c.c.}]\ . \quad (2)$$

Here ψ is the complex superconducting order parameter, $q=2e$ is the Cooper pair charge, and $\mathbf{A}$ is the vector potential whose curl yields the total magnetic field inside the superconductor.

$$\nabla\times\mathbf{A}=\mathbf{H}\ . \quad (3)$$

The mass tensor is diagonal with elements m_a,m_b,m_c in an orthogonal coordinate system having axes along crystallographic $\hat{\mathbf{a}},\hat{\mathbf{b}},\hat{\mathbf{c}}$ directions.

It is convenient to write (1) and (2) in terms of appropriately scaled lengths and magnetic fields. As usual, we introduce the average scalar mass $\overline{M}=|\det\overline{\overline{M}}|^{1/3}$, its inverse μ and the dimensionless tensors

$$\overline{\overline{m}}=\overline{\overline{M}}/\overline{M},\quad \overline{\overline{\mu}}=\overline{\overline{m}}^{-1}\ . \quad (4)$$

Following Abrikosov[6] we measure ψ in terms of the zero-field order parameter $|\psi_0|=\sqrt{|\alpha|/\beta}$, we measure lengths in terms of the London penetration depth $\lambda=(\overline{M}c^2/4\pi q^2|\psi_0|^2)^{1/2}$, and $\mathbf{H}$ in terms of the thermodynamic critical field $H_c\sqrt{2}$. Then

$$\mathbf{\Pi}\cdot\overline{\overline{\mu}}\cdot\mathbf{\Pi}\psi-\psi+|\psi|^2\psi=0\ , \quad (5)$$

$$\nabla\times\mathbf{H}=\overline{\overline{\mu}}/2\cdot(\psi^*\mathbf{\Pi}\psi+\text{c.c.})\ , \quad (6)$$

where $\mathbf{\Pi}\equiv(i\kappa)^{-1}\nabla-\mathbf{A}$ and $\kappa=\lambda/\xi$, with the coherence length $\xi\equiv\hbar/\sqrt{2\overline{M}|\alpha|}$.

We now undertake a further coordinate and field scaling which reduces GL1 to isotropic form in a scaled system with coordinates along orthogonal axes $\hat{\mathbf{e}}_1,\hat{\mathbf{e}}_2,\hat{\mathbf{e}}_3$. The transformations specified below were initially introduced by Klemm and Clem[4] in their treatment of the lower critical field of an anisotropic superconductor. In fact, these authors also employed their scaling technique near H_{c2}, but incorrectly evaluated the free energy there.

Let us specify real-space coordinates x,y,z such that z defines the direction of the vortex axis. Then the scaled coordinates q_1,q_2,q_3 are defined as

$$\mathbf{q}\equiv\overline{\overline{m}}^{1/2}\cdot\mathbf{x}\ . \quad (7)$$

If such a transformation is to be canonical, the momentum operator must scale in inverse fashion. Thus

$$\nabla_q\equiv\overline{\overline{\mu}}^{1/2}\cdot\nabla\ ,$$
$$\mathbf{a}\equiv\overline{\overline{\mu}}^{1/2}\,\mathbf{A}\ , \quad (8)$$
$$\boldsymbol{\pi}\equiv\overline{\overline{\mu}}^{1/2}\cdot\mathbf{\Pi}\ .$$

Then GL1 may be written in terms of scaled coordinates and operators as

$$\pi^2\psi-\psi+|\psi|^2\psi=0\ . \quad (9)$$

Equation (9) is manifestly isotropic, but to be useful it should also be true that $\mathbf{a}$ is related to an appropriately scaled magnetic field. This involves a trivial bit of algebra; one easily finds

$$\nabla_q\times\mathbf{a}=\mathbf{h}\ , \quad (10)$$

where the scaled magnetic field is defined as

$$\mathbf{h}\equiv\overline{\overline{m}}^{1/2}\cdot\mathbf{H}\ . \quad (11)$$

From (11) it also follows that

$$\nabla_q\cdot\mathbf{h}=\nabla\cdot\mathbf{H}=0\ . \quad (12)$$

Thus the scaled vector potential and magnetic field are related just as in unscaled space. Note, however, that if one defines the vector potential $\mathbf{A}$ in the Coulomb gauge, i.e., $\nabla\cdot\mathbf{A}=0$, then $\mathbf{a}$ will not satisfy this gauge condition in the scaled coordinate frame.

Note further that two invariants of such a transformation are the magnetic flux enclosed by a contour and the element of volume.

$$\Phi=\oint\mathbf{A}\cdot d\mathbf{x}=\oint\mathbf{a}\cdot d\mathbf{q} \quad (13)$$

and

$$dV=d\mathbf{z}\cdot(d\mathbf{x}\times d\mathbf{y})=d\mathbf{q}_3\cdot(d\mathbf{q}_1\times d\mathbf{q}_2)=dV_q\ . \quad (14)$$

The latter relation follows from the fact that $\det\overline{\overline{m}}=1$.

Before transforming the second GL equation, we remark that since the first equation has been transformed to isotropy, it follows that *any property of an anisotropic superconductor which depends only upon the first GL equation can be inferred from a scaling of the analogous isotropic result.* As one example of this property consider the angular dependence of the upper critical field for an arbitrary orthorhombic mass tensor. In the limit that $h\to h_{c2}$, $|\psi|^2\to0$ and we ignore the cubic term in (9). Then we have a linear Schrödinger-like equation for ψ which possesses a nonzero simple harmonic-oscillator solution only if $h<h_{c2}=\kappa$. Of course this is independent of the direction of $\mathbf{h}$, but upon scaling back to the laboratory coordinates, it leads to an angular dependence of H_{c2}. From (11)

$$h_{c2}^2=\mathbf{H}_{c2}\cdot\overline{\overline{m}}\cdot\mathbf{H}_{c2}=H_{c2}^2(\hat{\mathbf{z}}\cdot\overline{\overline{m}}\cdot\hat{\mathbf{z}})$$
$$=\mu H_{c2}^2(m_a\cos^2\alpha+m_b\cos^2\beta+m_c\cos^2\gamma)\ ,$$

where α,β,γ are the angles $\mathbf{H}_{c2}$ makes with the $\hat{\mathbf{a}},\hat{\mathbf{b}},\hat{\mathbf{c}}$ crystallographic axes. Thus the critical field is

$$H_{c2}(\alpha,\beta,\gamma)=\tilde{\kappa}$$
$$\equiv\kappa[\mu(m_a\cos^2\alpha+m_b\cos^2\beta+m_c\cos^2\gamma)]^{-1/2} \quad (15)$$

a result which reduces to the well-known uniaxial case[5] if $m_a=m_b$. Equation (15) also appears in Ref. 4 although its presence does not seem to have been widely appreciated since this work deals primarily with anisotropy in H_{c1}.

Although the mass tensor cannot be transformed out of the second Ginzburg-Landau equation, it is nevertheless useful to write this equation in scaled space. To do this we introduce the scaled current density $\mathbf{j}$

$$\mathbf{j}\equiv\overline{\overline{m}}^{1/2}\cdot\mathbf{J}\ . \quad (16)$$

From (16) it follows that the divergence of the current density vanishes in both coordinate systems.

$$\nabla\cdot\mathbf{J}=\nabla_q\cdot\mathbf{j}=0\ . \tag{17}$$

Inserting (16) into GL2 and transforming the curl and magnetic field to the scaled frame, the second Ginzburg-Landau equation becomes

$$\nabla_q\times\mathbf{h}'=\tfrac{1}{2}(\psi^*\boldsymbol{\pi}\psi+\text{c.c.})\ . \tag{18}$$

Here $\mathbf{h}'$ is yet another auxiliary scaled field defined as

$$\mathbf{h}'=\overline{\overline{\mu}}\cdot\mathbf{h}=\overline{\overline{\mu}}^{1/2}\cdot\mathbf{H}\ . \tag{19}$$

In the terminology of Ref. 3, $\mathbf{h}'$ and $\mathbf{h}$ are the covariant and contravariant fields corresponding to $\mathbf{H}$. Note that although (18) is written in a form which superficially makes it appear that the mass tensor has scaled out, this is not really so. In particular we will later see that the appearance of $\mathbf{h}'$ rather than $\mathbf{h}$ in (18) results in such effects as the existence of internal magnetic field components which point perpendicular to a vortex axis.[1-3,7]

Finally let us pause to clarify the geometry of the scaling transformation. There are three sets of orthogonal axes of interest. The absolutely fixed set is defined by the crystallographic axes $\hat{\mathbf{a}},\hat{\mathbf{b}},\hat{\mathbf{c}}$. This is often the most convenient set in which to calculate, and both of the other sets are defined relative to it. The matrix equation (7) has its simplest form when expressed in this frame, i.e.,

$$\begin{aligned} q_a&=\sqrt{\mu m_a}x_a\ ,\\ q_b&=\sqrt{\mu m_b}x_b\ ,\\ q_c&=\sqrt{\mu m_c}x_c\ . \end{aligned} \tag{20}$$

The second set is the unscaled coordinate frame in which the z axis defines the direction of the vortices. Vortices in a uniaxial crystal are frequently taken to lie in the x-z plane, inclined by angle θ to the c axis. The third set has its three axis defined by the *scaled* vortex direction. For a uniaxial superconductor the scaled vortices would then lie in the scaled 1-3 plane inclined by angle θ' to the c axis. The relation between these two angles follows from the field transformation equations

$$\tan\theta'=\sqrt{m_a/m_c}\tan\theta\ . \tag{21}$$

For large anisotropy this relation implies that θ' is quite small for most external field orientations. This geometry is illustrated in Fig. 1.

Although we have not yet explored the GL solutions for the currents and fields, it is useful to anticipate later results in order to show how our scaled coordinates are related to the nonorthogonal coordinate system introduced by Kogan and Clem.[3] These authors introduced a system in which their z axis also defined the external field direction, while the other two coordinates lay in a nonorthogonal plane which carried the supercurrents. Because of the anisotropy, they showed that the normal to this current plane was tilted by an angle $\phi\neq 0$ from the field direction.

Now we shall later show that in our scaled coordinate system, as in the isotropic case, the scaled supercurrents induced by the external field $\mathbf{h}_0=h_0\hat{\mathbf{e}}_3$, *do* flow in a plane perpendicular to $\mathbf{h}_0$. Thus

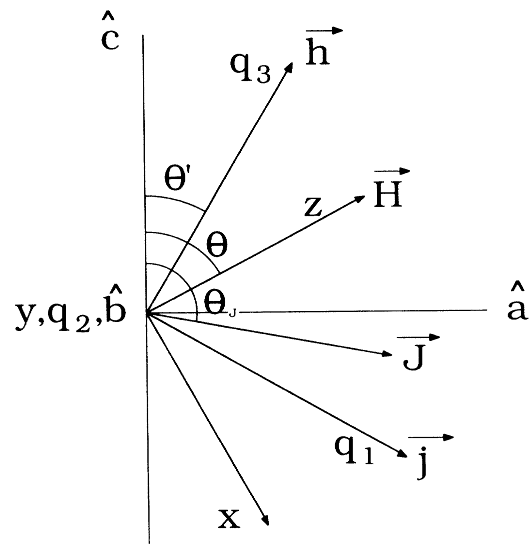

FIG. 1. The geometry of the three coordinate systems in the text for $m_c/m_a=10$ and $\theta'=30°$ in a uniaxial crystal. Scaled and real current planes are also indicated. Relative lengths of h,H, and j,J are drawn to scale.

$$\mathbf{j}\cdot\mathbf{h}_0=0=\mathbf{J}\cdot\overline{\overline{m}}\cdot\mathbf{H}_0\ . \tag{22}$$

As found in Ref. 3, (22) makes it clear that $\mathbf{J}\cdot\mathbf{H}_0\neq 0$ in the presence of anisotropy. Expressing this equation in terms of crystallographic axes we have for uniaxial symmetry with $H_b=0$,

$$J_aH_am_a+J_cH_cm_c=0\ . \tag{23}$$

We define $H_a=H\sin\theta$, $H_c=H\cos\theta$, $J_a=J\sin\theta_J$, $J_c=J\cos\theta_J$. Then Eq. (21) implies

$$\tan\theta_J=-(m_c/m_a)\cot\theta\ . \tag{24}$$

The angle $\phi=\pi/2-(\theta_J-\theta)$ is the tilt angle of Kogan and Clem. Thus using (24) to eliminate θ_J we easily recover

$$\tan\phi=\tan\theta\left[\frac{m_c-m_a}{m_c+m_a\tan^2\theta}\right]\ , \tag{25}$$

which is Eq. (33) of Ref. 3. We conclude that the 1-2 current plane of our scaled coordinate frame transforms into the nonorthogonal current plane of Kogan and Clem in real space. The real and scaled current planes are also illustrated in Fig. 1.

It is also possible to give a very intuitive picture of the behavior of anisotropic superconductors which illustrates why the scaling transformation is so useful. The first Ginzburg-Landau equation resembles a Schrödinger equation for a particle with an ellipsoidal constant-energy surface $\varepsilon_k=\frac{1}{2}\hbar^2\mathbf{k}\cdot\overline{\overline{\mu}}\cdot\mathbf{k}$, and which is subject to an external magnetic field $\mathbf{H}_0$ tipped relative to the principal axes of the ellipsoid. In a semiclassical approximation, it is well known that current carried by states in the plane defined by $\mathbf{k}\cdot\mathbf{H}_0=0$ lies not in the $\mathbf{k}$ plane, but in the plane defined by the velocity $\mathbf{v}_k$.

$$\mathbf{J} \propto \mathbf{v}_k = (1/\hbar)\nabla_k \varepsilon_k = \hbar \bar{\bar{\mu}} \cdot \mathbf{k} \ . \tag{26}$$

Multiplying (26) by $\bar{\bar{m}}$, and taking the scalar product with $\mathbf{H}_0$, we recover precisely (22). Thus the current plane of the GL theory is also defined by (26). The point of the scaling transformation is then that it converts the constant energy ellipsoid to a sphere. In so doing the direction of the scaled field is altered, and the scaled diamagnetic current response does lie in a plane which is perpendicular to this scaled field, as also in the isotropic case.

III. SOLUTION OF THE SCALED EQUATIONS

Consider the first GL equation (9) in scaled space. We will work through relatively well established techniques of its solution[3,6] so that the deviations from these for the anisotropic case are clearly seen. We first define the operators $\pi^{\pm} = \pi_1 \pm i\pi_2$. The commutator is readily found.

$$i[\pi_1, \pi_2] = -h_3/\kappa = -h_3/h_{c2} \ . \tag{27}$$

Thus (9) may be written as

$$\pi^- \pi^+ \psi = -\pi_3^2 \psi + (1 - h_3/h_{c2})\psi - |\psi|^2 \psi \ . \tag{28}$$

Each term on the right side of (28) is small near h_{c2} so that if $\psi = \psi_0 + \psi_1$ the zero-order solution ψ_0 satisfies

$$\pi^+ \psi_0 = 0 \ , \tag{29}$$

and ψ_1 obeys

$$\pi^- \pi^+ \psi_1 = (1 - h_3/h_{c2})\psi - |\psi|^2 \psi - \pi_3^2 \psi \ . \tag{30}$$

Thus the possible solutions $\psi_0(\mathbf{q})$ in scaled space will have exactly the same form as they do in the case of an isotropic superconductor.

Consider now the current associated with this zero-order solution. For $\psi_0 = |\psi_0| e^{i\chi}$ one finds

$$\mathbf{j} = |\psi_0|^2 [(1/\kappa)\nabla_q \chi - \mathbf{a}] \ . \tag{31}$$

Since $|\psi_0|^2$ is already first order small near h_{c2}, (31) implies that j_3 may be neglected compared to j_1 and j_2. Thus the current response in scaled space is perpendicular to the applied field, as stated earlier. By equating the real and imaginary parts of (29) to zero one also finds

$$j_1 = -\frac{1}{2\kappa} \frac{\partial |\psi_0|^2}{\partial q_2} ; j_2 = \frac{1}{2\kappa} \frac{\partial |\psi_0|^2}{\partial q_1} \ . \tag{32}$$

All of the preceding equations are exactly the same as for an isotropic superconductor, but at this point differences emerge from the fact that it is $\mathbf{h}'$ and not $\mathbf{h}$ which appears in GL2. Noting that $\mathbf{j}$ can be written as a curl, one is tempted to set $\mathbf{h}_s' = -(|\psi_0|^2/2\kappa)\hat{\mathbf{e}}_3$, where $\mathbf{h}_s'$ is the diamagnetic field due to the supercurrents only. While this satisfies (18), it would also imply that the divergence of $\mathbf{h}_s'$ is zero—a result at variance with the requirement that the divergence of $\mathbf{h}_s$ be zero. In order to satisfy this latter equation as well as (18), an additional term must be added to $\mathbf{h}_s'$. This correction takes the form of a gradient so that it does not affect $\mathbf{j}$. However, it does render the divergence of $\mathbf{h}_s$ zero, and also contributes to the existence of internal fields perpendicular to the vortex axis.

In the Appendix we outline the calculation of this correction term and quote only the result here.

$$\mathbf{h}_s' = -\frac{|\psi_0|^2}{2\kappa} \hat{\mathbf{e}}_3 - \frac{1}{8\pi\kappa} \nabla_q (\hat{\mathbf{e}}_3 \cdot \bar{\bar{m}} \cdot \nabla_q I) \ , \tag{33}$$

where we define the integral,

$$I \equiv \int dV' \frac{|\psi_0(\mathbf{x}')|^2}{|\mathbf{x} - \mathbf{x}'|} = \int dV_q' \frac{|\psi_0(\mathbf{q}')|^2}{|\mathbf{x} - \mathbf{x}'|} \ . \tag{34}$$

In the second form we have used the invariance of the volume element to note that the integral may be evaluated in either real or scaled space. The actual scaled field $\mathbf{h}_s$ is easily found by multiplying (33) by $\bar{\bar{m}}$. Further noting that $\nabla^2 = \nabla_q \cdot \bar{\bar{m}} \cdot \nabla_q$ it is readily checked that $\nabla_q \cdot \mathbf{h}_s = 0$, since

$$\nabla^2 I = -4\pi |\psi_0|^2 \ . \tag{35}$$

The actual physical field $\mathbf{H}_s$ is

$$\begin{aligned} \mathbf{H}_s &= \frac{-1}{2\kappa} |\psi_0|^2 \bar{\bar{m}}^{1/2} \cdot \hat{\mathbf{e}}_3 - \frac{1}{8\pi\kappa} \nabla(\hat{\mathbf{e}}_3 \cdot \bar{\bar{m}}^{1/2} \cdot \nabla I) \\ &= -\frac{\tilde{\kappa}}{2\kappa^2} |\psi_0|^2 \bar{\bar{m}} \cdot \hat{\mathbf{z}} - \frac{\tilde{\kappa}}{8\pi\kappa^2} \nabla(\hat{\mathbf{z}} \cdot \bar{\bar{m}} \cdot \nabla I) \ . \end{aligned} \tag{36}$$

The component of $\mathbf{H}_s$ along the direction of the applied field is

$$H_{sz} = -\frac{\tilde{\kappa}}{2\kappa^2} |\psi_0|^2 \hat{\mathbf{z}} \cdot \bar{\bar{m}} \cdot \hat{\mathbf{z}} = -|\psi_0|^2 / 2\tilde{\kappa} \ , \tag{37}$$

a result equivalent to Eq. (51) of Kogan and Clem.[3] Thus while the gradient correction term in (36) does not contribute to H_{sz} since $\partial I/\partial z = 0$, it does give rise to transverse field components which complicate the determination of the vortex lattice structure.

In order to find the lattice geometry we need to derive the appropriate normalization condition for the order parameter. To leading order ψ on the right side of (28) may be replaced by ψ_0 and the π_3 term may be dropped. Then multiplying through by ψ_0^* on the left, integrating over the volume, and using the Hermitian property of $\pi^{\pm}$ we recover

$$0 = \overline{(1 - h_3/h_{c2})|\psi_0|^2} - \overline{|\psi_0|^4} \ . \tag{38}$$

With $h_3 = h_0 + h_{s3}$ we have

$$0 = (1 - h_0/h_{c2})\overline{|\psi_0|^2} - \overline{h_{s3}|\psi_0|^2}/\kappa - \overline{|\psi_0|^4} \ . \tag{39}$$

While this superficially looks like the result for an isotropic system, it really is not, since the expression for h_{s3} is considerably more complicated.

$$h_{s3} = -\frac{1}{2\kappa} |\psi_0|^2 \hat{\mathbf{e}}_3 \cdot \bar{\bar{m}} \cdot \hat{\mathbf{e}}_3 - \frac{1}{8\pi\kappa} (\hat{\mathbf{e}}_3 \cdot \bar{\bar{m}} \cdot \nabla_q)^2 I \ . \tag{40}$$

For an isotropic system the last term vanishes, but in an anisotropic system it is proportional to finite off-diagonal matrix elements of the mass tensor.

Note finally that in (39) we may replace $|\psi_0|^2$ in the second term using (33) so that

$$0=(1-h_0/h_{c2})\overline{|\psi_0|^2}+2\overline{h_{s3}h'_{s3}}-\overline{|\psi_0|^4} . \tag{41}$$

The last two terms also appear in the free energy as we shall see.

The reduced free energy in real space, after a parts integration is[3]

$$F=\overline{H^2}-\tfrac{1}{2}\overline{|\psi_0|^4} . \tag{42}$$

If we wish to represent this in scaled space we may also write

$$F=\overline{\mathbf{h}\cdot\mathbf{h}'}-\tfrac{1}{2}\overline{|\psi_0|^4} . \tag{43}$$

Following Abrikosov[6] we wish to express F in terms of the magnetic induction $\mathbf{B}$ or its scaled counterpart $\mathbf{b}=(\overline{\overline{m}})^{1/2}\cdot\mathbf{B}$. We define

$$\begin{aligned}\mathbf{B}&=\mathbf{H}_0+\overline{H_s} ,\\ \mathbf{b}&=\mathbf{h}_0+\overline{h_s} .\end{aligned} \tag{44}$$

Kogan and Clem[3] have shown that the average diamagnetic field perpendicular to the vortex axis is zero. Exactly equivalent arguments in scaled space lead to the conclusion that only the average component $\overline{h_{s3}}$ is nonzero. Thus

$$\begin{aligned}B&=H_0+\overline{H_{sz}},\ \overline{H_{sx}}=\overline{H_{sy}}=0\\ b&=h_0+\overline{h_{s3}},\ \overline{h_{s1}}=\overline{h_{s2}}=0 ,\end{aligned} \tag{45}$$

where from (37)

$$\begin{aligned}\overline{H_{sz}}&=-\overline{|\psi_0|^2}/2\tilde{\kappa} ,\\ \overline{h_{s3}}&=\overline{H_{sz}}(\kappa/\tilde{\kappa}) .\end{aligned} \tag{46}$$

Returning to (38) we derive the normalization of ψ_0 as a function of b in scaled space.

$$0=(1-b/h_{c2})\overline{|\psi_0|^2}-\overline{(h_{s3}-\overline{h_{s3}})|\psi_0|^2}/\kappa-\overline{|\psi_0|^4} . \tag{47}$$

The last two terms are quadratic in $|\psi_0|^2$ while the first is linear. After dividing by $(\overline{|\psi_0|^2})^2$, the former are independent of the normalization, and we solve for $\overline{|\psi_0|^2}$.

$$\overline{|\psi_0|^2}=(h_{c2}-b)/(\kappa\beta_A+g/\kappa) . \tag{48}$$

β_A is the usual Abrikosov parameter and the function g is defined as

$$g\equiv\kappa\overline{(h_{s3}-\overline{h_{s3}})|\psi_0|^2}/(\overline{|\psi_0|^2})^2 . \tag{49}$$

This function, which also appears in the free energy, determines the structure and geometry of the vortex lattice. In the isotropic limit it is proportional to β_A-1.

Returning to the free energy (42), a short exercise suffices to show that

$$\overline{h_1h'_1}+\overline{h_2h'_2}=0 . \tag{50}$$

Thus, on average, the perpendicular components of the two scaled fields are orthogonal. Then the free energy becomes

$$\begin{aligned}F&=\overline{h_3h'_3}-\tfrac{1}{2}\overline{|\psi_0|^4}\\ &=\overline{[\overline{h}_3+(h_3-\overline{h}_3)]h'_3}-\tfrac{1}{2}\overline{|\psi_0|^4}\\ &=B^2+\overline{(h_{s3}-\overline{h}_{s3})h'_{s3}}-\tfrac{1}{2}\overline{|\psi_0|^4} .\end{aligned} \tag{51}$$

In the last form the first term is rewritten for simplicity as the square of the magnetic induction in real space. Note that the last two terms also appear in the normalization condition, so that

$$\begin{aligned}F&=B^2-\tfrac{1}{2}(1-b/h_{c2})\overline{|\psi_0|^2}\\ &=B^2-\tfrac{1}{2}(h_{c2}-b)^2/(\kappa^2\beta_A+g) .\end{aligned} \tag{52}$$

Equation (52) is our final result for the free energy. It is valid for any lattice geometry with vortices aligned along $\hat{\mathbf{e}}_3$ (or $\hat{\mathbf{z}}$). We shall determine the lowest energy geometry shortly, but pause first to generalize a result, first noted by Kogan and Clem,[3] involving the magnetization of the superconductor. It is of interest because it is independent of the detailed structure of the vortex lattice.

In the numerator of the condensation energy we have

$$\begin{aligned}(h_{c2}-b)^2&=(\mathbf{h}_{c2}-\mathbf{b})\cdot(\mathbf{h}_{c2}-\mathbf{b})\\ &=(\mathbf{H}_{c2}-\mathbf{B})\cdot\overline{\overline{m}}\cdot(\mathbf{H}_{c2}-\mathbf{B}) .\end{aligned} \tag{53}$$

Now the macroscopic thermodynamic field is

$$\begin{aligned}\mathbf{H}&=\tfrac{1}{2}\nabla_B F\\ &=\mathbf{B}-\tfrac{1}{2}\overline{\overline{m}}\cdot(\mathbf{B}-\mathbf{H}_{c2})/(\kappa^2\beta_A+g) .\end{aligned} \tag{54}$$

Thus the bulk magnetization is

$$\mathbf{M}=\frac{\mathbf{B}-\mathbf{H}}{4\pi}=\frac{-1}{8\pi}\overline{\overline{m}}\cdot(\mathbf{H}_{c2}-\mathbf{B})/(\kappa^2\beta_A+g) . \tag{55}$$

If we project $\mathbf{M}$ along the principal axes we find

$$\begin{aligned}M_a&=km_a(\hat{\mathbf{a}}\cdot\hat{\mathbf{n}}) ,\\ M_b&=km_b(\hat{\mathbf{b}}\cdot\hat{\mathbf{n}}) ,\\ M_c&=km_c(\hat{\mathbf{c}}\cdot\hat{\mathbf{n}}) ,\end{aligned} \tag{56}$$

where $\hat{\mathbf{n}}$ is a unit vector pointing along $\mathbf{H}_{c2}-\mathbf{B}$ and where the constant k is the same for all three components. For small magnetization the vector $\hat{\mathbf{n}}$ points along the external field direction. Thus

$$\begin{aligned}M_a&=km_a\cos\alpha ,\\ M_b&=km_b\cos\beta ,\\ M_c&=km_c\cos\gamma ,\end{aligned} \tag{57}$$

where α,β,γ are the same angles defined in (15). Then the ratios of any two of these components are independent of the lattice geometry and the maximum magnetization tends to be along the high mass direction. In the special uniaxial case with the external field in the a-c plane, $M_b=0$ and

$$\frac{M_a}{M_c}=\frac{m_a}{m_c}\tan\theta , \tag{58}$$

which is Eq. (75) of Ref. 3. A similar relation was found by Campbell *et al.*[1] in the London limit of uniaxial anisotropy.

Referring back to Eqs. (22) and (55), we see that the origin of such simple relationships is the intuitively obvious fact that the current plane and the bulk magnetization are perpendicular, i.e., $\mathbf{J}\cdot\mathbf{M}=0$. This must hold independent of the flux line lattice geometry.

We return to (52) to determine the lowest energy lattice geometry. Clearly we need to minimize the denominator. It is convenient to express D in reciprocal space.

$$D=2\kappa^2\sum_G|\omega_G|^2+2\kappa\sum_G{}' h_{s3}(G)\omega_{-G} \ , \tag{59}$$

where ω_G is the Fourier transform of $|\psi_0|^2$, normalized to $\omega_0=1$. The summation is over a complete set of reciprocal lattice vectors in scaled space, and the primed summation omits the $G=0$ term.

From (40) the Fourier transform of h_{s3} is easily evaluated in scaled space. Inserting it into D above we find

$$D=2\kappa^2\beta_A-\sum_G{}'|\omega_G|^2[m_{33}-(\hat{\mathbf{e}}_3\cdot\overline{\overline{m}}\cdot\mathbf{G})^2/(\mathbf{G}\cdot\overline{\overline{m}}\cdot\mathbf{G})] \ , \tag{60}$$

where $m_{ij}=\hat{\mathbf{e}}_i\cdot\overline{\overline{m}}\cdot\hat{\mathbf{e}}_j$. Notice that the only term which connects the vortex lattice to the underlying crystal is the second one in brackets, because it depends upon matrix elements of the mass tensor between the field direction and the direction of the reciprocal lattice. In the absence of this term, it is clear that the structure of the lattice is the usual triangular lattice in scaled space which minimizes β_A and hence D.

Also, for large values of κ it is clear that $2\kappa^2\beta_A\gg1$ so that the equilibrium lattice must be the triangular lattice or something very close to it. The last term then serves only to orient this lattice with respect to crystalline axes.

To see how this is accomplished, consider a uniaxial case, with the vortex axis in the a-c plane. Then $m_{32}=m_{12}=0$ so the denominator D may be written as

$$D=2\kappa^2\beta_A-m_{33}(\beta_A-1)+\sum_G{}'|\omega_G|^2\left[\frac{m_{31}^2G_1^2}{m_{11}G_1^2+m_{22}G_2^2}\right] \ , \tag{61}$$

where $\beta_A-1=\sum_G'|\omega_G|^2\approx0.16$ for the hexagonal lattice.[8] Thus the equilibrium orientation will minimize the last term. To an excellent approximation for any hexagonal lattice we can factor it as β_A-1 times an angular function $f(\phi)$ where

$$f(\phi)\equiv\tfrac{1}{6}\sum_G{}'\frac{m_{31}^2G_1^2}{m_{11}G_1^2+m_{22}G_2^2} \ . \tag{62}$$

We define the angle ϕ as the angle between the $\hat{\mathbf{e}}_1$ axis and the closest of the six smallest reciprocal lattice vectors and do the summation above only over these vectors. The factorization follows since the G sum is completely dominated by this reduced set,[8] in which each vector has an identical $|\omega_G|^2$. For example, such an approximation represents β_A-1 to better than 0.1%.

A plot of $f(\phi)$ for several different asymmetry parameters

$$A(\theta')\equiv m_{11}/m_{22}=\cos^2\theta'+(m_c/m_a)\sin^2\theta'$$

is shown in Fig. 2. In each case the equilibrium lattice is found to have $\phi=30°$. Of course this corresponds to a direct vortex lattice which is rotated by 30° from its reciprocal lattice. When translated back to real space this lattice has just the orientation which has been found by Campbell *et al.*[1] in the London limit.

From the form of $f(\phi)$ it is not difficult to discover why $\phi=30°$ is preferred. At this orientation, two of the six smallest reciprocal lattice vectors lie along the $\hat{\mathbf{e}}_2$ direction and do not contribute to it at all. In the other symmetrical orientation, $\phi=0°$, where one might expect an extremum, one finds a maximum of $f(\phi)$. A bit of algebra enables one to show analytically that $f(0°)-f(30°)\geq0$ for *any* choice of asymmetry. This is universally true for either $m_c>m_a$ or $m_a>m_c$.

One other point to note is that as the scaled field direction approaches either the a or c axis the minimum of $f(\phi)$ becomes increasingly shallow. This reflects the fact that the free energy is independent of ϕ if $\hat{\mathbf{e}}_3$ lies exactly along a principal axis of the mass tensor. Mathematically since $m_{31}=0$, the last term in (61) vanishes so that the entire energy denominator is rotationally invariant. When translated back to real space, this leads to an infinite number of geometrically inequivalent but energetically equivalent lattices.[1]

In fact such a result is universally valid for an *arbitrary*

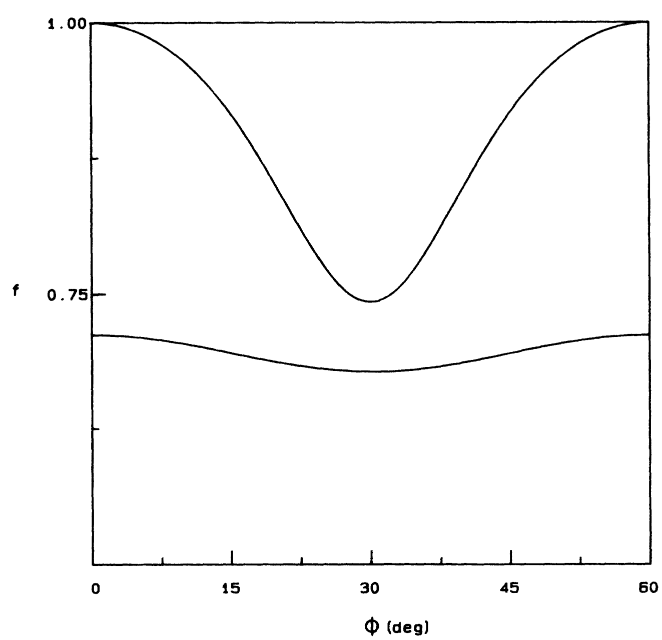

FIG. 2. The orientation function $f(\phi)$ of the triangular lattice as a function of the relative orientation of the scaled one axis and the reciprocal lattice. The universal minimum energy occurs at $\phi=30°$. The curves correspond to $m_c/m_a=25$ and $\theta'=45°$ (upper) and 11.8° (lower) with asymmetries $A=13{,}2$, respectively.

nonuniaxial mass tensor. This follows from (60) since if $\mathbf{H}$ points along a principal axis, so do $\mathbf{h}$ and $\hat{\mathbf{e}}_3$. But then $\hat{\mathbf{e}}_3\cdot\overline{\overline{m}}\cdot\mathbf{G}=m_{33}\hat{\mathbf{e}}_3\cdot\mathbf{G}=0$ because $\mathbf{G}$ has nonvanishing components only in the 1-2 plane. D and the free energy are then invariant under rotations about the three-axis.

While the equilibrium lattice is clearly triangular with $\phi=30°$ in the high κ limit, it seems likely that if κ is relatively small (much smaller than characteristic of HTSC's), significant distortions may occur. In this regime, the last term in (61) becomes more comparable to the others. It is important to note that *by itself* this term will not be minimized by a triangular lattice. Thus it is reasonable to expect its interplay with the rotationally invariant terms to result in distortions of the triangular lattices. Such distortions may be expected to be $O(\kappa^{-2})$ and will be discussed more fully in a future publication.

Consider now the internal magnetic fields of the large κ equilibrium triangular lattice. We have already noted that the field h'_{s3} is proportional to $|\psi_0|^2$. Thus contours of constant $|\psi_0|^2$ are also contours of constant h'_{s3}. In real-space equation (37) shows that contours of constant $|\psi_0|^2$ are also contours of H_{sz}. Except for the geometry, this is analogous to results for the isotropic case.

A fundamental difference of the anisotropic case involves the existence of transverse fields $h_{1,2}(q_1,q_2)$. Such fields have recently been experimentally documented by the torque measurements of Farrell *et al.*[9] Since the divergence of $\mathbf{h}$ vanishes and $\mathbf{h}=\mathrm{curl}_q\mathbf{a}$, we can identify the transverse field lines as contours of constant a_3, where in the uniaxial limit,

$$a_3=\frac{m_{31}m_{22}}{8\pi\kappa}\frac{\partial I}{\partial q_2}=-\left[\frac{\overline{M}}{m_a}-\frac{\overline{M}}{m_c}\right]\frac{\sin\theta'\cos\theta'}{8\pi\kappa}\frac{\partial I}{\partial q_2}\ . \tag{63}$$

It is clear that $a_3=0$ for the case of isotropy ($m_a=m_c$), or for the cases that the external field points along a symmetry axis ($\theta'=0,\theta'=\pi/2$). The maximum transverse field occurs around $\theta'=45°$.

To illustrate the nature of this field we have plotted in

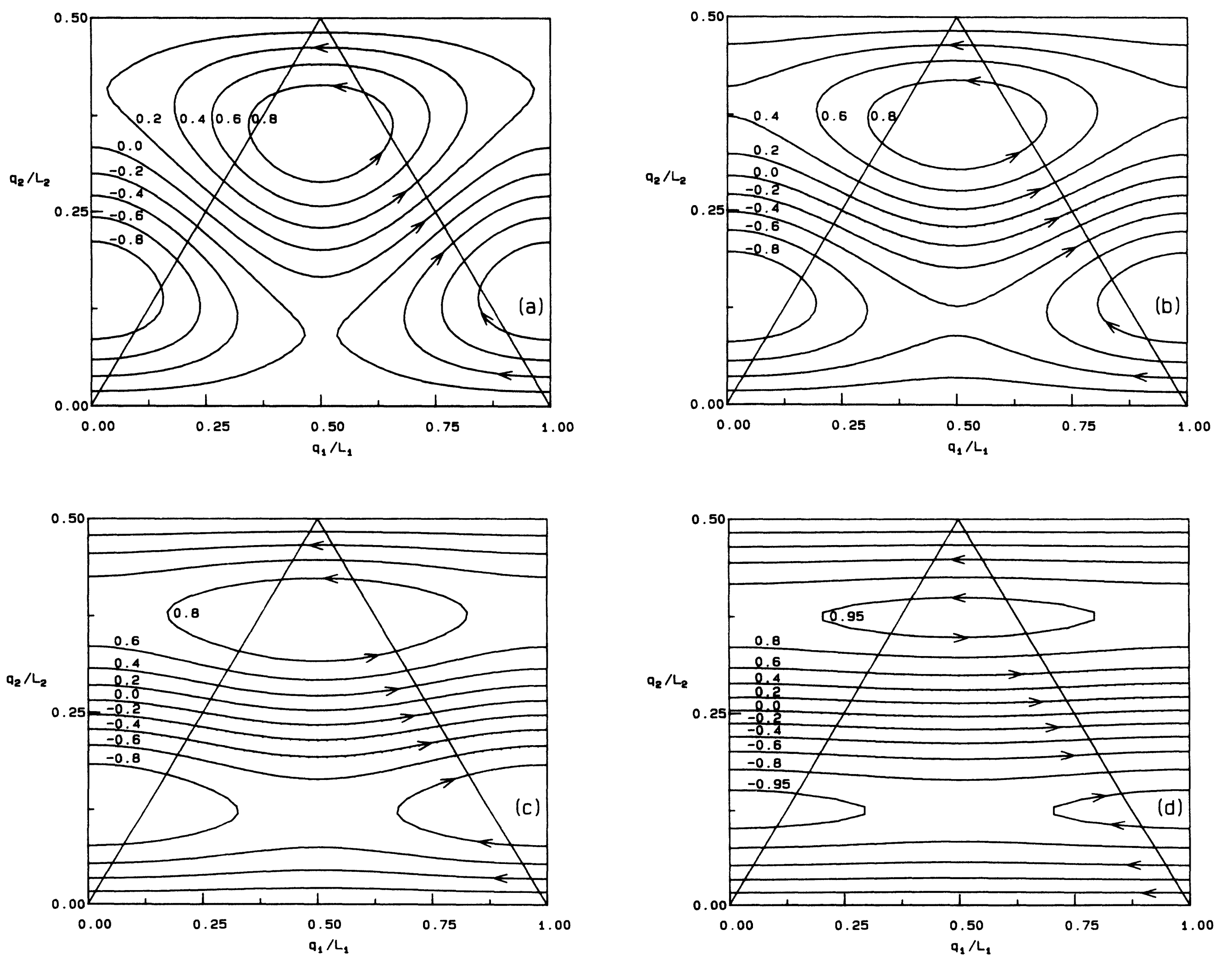

FIG. 3. The lines of the transverse field plotted in the scaled coordinate frame for four different values of the anisotropy parameter $A(\theta')$ defined in the text. (a) $A=1$ (the field amplitude is zero for this case), (b) $A=2$, (c) $A=6$, (d) $A=25$. In all cases the border lines $q_2=0,0.5L_2$ are also field lines. Numbers attached to the contours represent values of a_3 normalized to unity at $(0,L_2/8)$.

Fig. 3 the field line geometry for the case of uniaxial anisotropy, and for various asymmetries A. In doing so we have dropped the prefactor in equation (63) and plotted only $\partial I/\partial q_2$ so that the isotropic field lines ($m_a=m_c$) can also be shown. Increasing anisotropy can then be seen as a distortion of these fundamental lines. Our plots are done in the invariant scaled space and utilize the conventions of Kleiner *et al.*[8] Thus there are two vortices per rectangular unit cell having dimensions $L_2/L_1=\sqrt{3}$. The vortices are situated at the corners of the equilateral triangle with spacing L_1.

The first notable feature is that the transverse field breaks the sixfold rotational symmetry of the vortex geometry. The field lines are invariant only under a 180° rotation around a vortex. This is to be expected since the transverse field results from a coupling of the underlying tetragonal symmetry of the crystal lattice to the hexagonal symmetry of the vortex array.

Secondly, one finds regions in each triangular cell in which the field lines close upon themselves (islands) interspersed by other regions in which the field flows continuously along the $\hat{\mathbf{e}}_1$ axis. There is always one zero of the field located at the center of these islands on the lines $q_1=\frac{1}{2}nL_1$. As the asymmetry increases, the size of these island regions decreases; and the islands flatten. In the limit of extreme anisotropy, $m_a/m_c\to 0$ and the field contours become identical with lines of constant q_2, with $h_2\approx 0$.

IV. SUMMARY AND CONCLUSIONS

We have applied a coordinate and field scaling technique to the solution of the Ginzburg-Landau equations appropriate to an anisotropic superconductor near its upper critical field. This scaling results in a number of clear parallels and differences between the isotropic and anisotropic cases.

(1) The scaling renders the first GL equation completely isotropic, so that all known isotropic results which depend only upon it may be scaled into the anisotropic case. As examples of this we have the angular dependence of H_{c2} and the form of the zero-order ψ_0 solution.

(2) The scaled ground-state current density is derived from ψ_0 exactly as in the isotropic case, cf., Eq. (32). Although the scaled currents flow in a plane perpendicular to the direction of the scaled external field, the actual unscaled currents and fields are tilted from perpendicularity.[3] The amount of this tilt can be quantitatively found by a semiclassical analogy involving a particle having an ellipsoidal constant energy surface and subject to an external field. The bulk magnetization is perpendicular to this tilted current plane.

(3) The normalization condition for ψ_0, Eq. (39), is also implicitly analogous to the isotropic result except that the internal field h_{s3} bears a more complicated relationship (40) to the order parameter. This leads finally to an expression for the condensation energy which depends not only upon the Abrikosov β_A, but also upon the orientation of the flux-line lattice relative to the underlying crystallographic axes.

We can make this point more explicit by recasting the energy in terms of a correction to the isotropic result. After a bit of algebra one can write the condensation energy for the uniaxial case in real space as

$$F_s=-(H_{c2}-B)^2/D'$$

$$D'=\left[\frac{\tilde{\kappa}}{\kappa}\right]^2 D=1+(2\tilde{\kappa}^2-1)\beta_A - A^2\sin^2\theta\cos^2\theta\left[1-\frac{m_a}{m_c}\right]^2\sum_G{}'\frac{|\omega_G|^2G_2^2}{G_2^2+G_1^2A} . \quad (64)$$

Here

$$A(\theta)=(\cos^2\theta+m_a/m_c\sin^2\theta)^{-1}$$

is the former asymmetry parameter rewritten in terms of real-space angles. The last term above is the sole correction to the usual form of the isotropic energy, expressed in terms of an effective $\tilde{\kappa}$ value. This term, missed in the analysis of Ref. 4, is responsible for tying the flux lattice to the crystal. Under circumstances where $\tilde{\kappa}$ is relatively large, the correction is small and the flux lattice is an oriented equilateral triangular lattice in scaled space.

(4) One of the distinguishing features of anisotropic superconductors is the presence of their transverse internal fields. These have been graphed in Fig. 3 under varying conditions of anisotropy. It is noteworthy that they are at least qualitatively very similar to the fields calculated by Thiemann *et al.*[10] in the London approximation. Although these authors did not present as many cases of anisotropy, the resemblance between our two calculations is unmistakable, e.g., the presence in both of field islands with an associated field zero at corresponding positions. We conclude that there appears to be relatively little qualitative difference between a high-field GL theory and the lower field London theory. Both the lattice orientations and internal fields are quite similar. The primary difference would seem to be the relative sizes of the transverse and longitudinal fields.

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APPENDIX

We derive here the solutions for the internal magnetic fields and their associated vector potentials. We start with the solution for the vector potential in the second GL equation in real space

$$\mathbf{A}_s=\frac{1}{4\pi}\int\frac{\mathbf{J}dV'}{|\mathbf{x}-\mathbf{x}'|} , \quad (A1)$$

where we assume the Coulomb gauge is taken. Substituting for the scaled potential and current yields

$$\mathbf{a}_s=\frac{\bar{\bar{\mu}}}{4\pi}\cdot\int\frac{\mathbf{j}dV_q'}{|\mathbf{x}-\mathbf{x}'|} , \quad (A2)$$

where we have used our freedom to express both $\mathbf{j}$ and the volume element in scaled space. Applying Eq. (32) and performing a parts integration leads to

$$\mathbf{a}_s = \frac{\overline{\overline{\mu}}}{8\pi\kappa} \cdot \left[\hat{\mathbf{e}}_1 \frac{\partial I}{\partial q_2} - \hat{\mathbf{e}}_2 \frac{\partial I}{\partial q_1} \right] , \tag{A3}$$

where I is defined in (34).

The scaled internal field $\mathbf{h}_s$ is found by taking the curl of $\mathbf{a}_s$. In so doing it is important to notice that there exists a nonzero longitudinal component a_3 of the vector potential. One finds

$$h_{s1} = \frac{\partial a_3}{\partial q_2} = \frac{1}{8\pi\kappa} \left[\mu_{32} \frac{\partial^2 I}{\partial q_1 \partial q_2} - \mu_{31} \frac{\partial^2 I}{\partial q_1^2} \right] ,$$

$$h_{s2} = -\frac{\partial a_3}{\partial q_2} = \frac{1}{8\pi\kappa} \left[\mu_{31} \frac{\partial^2 I}{\partial q_1 \partial q_2} - \mu_{32} \frac{\partial^2 I}{\partial q_1^2} \right] , \tag{A4}$$

$$\begin{aligned} h_{s3} &= \frac{\partial a_2}{\partial q_1} - \frac{\partial a_1}{\partial q_2} \\ &= \frac{1}{8\pi\kappa} \left[\mu_{22} \frac{\partial^2 I}{\partial q_1^2} + \mu_{11} \frac{\partial^2 I}{\partial q_2^2} - 2\mu_{12} \frac{\partial^2 I}{\partial q_1 \partial q_2} \right] , \end{aligned}$$

where $\mu_{ij} \equiv \hat{\mathbf{e}}_i \cdot \overline{\overline{\mu}} \cdot \hat{\mathbf{e}}_j = \mu_{ji}$ in the scaled system. Equations (A4) are not very transparent. Their meaning is clearer if we use them to find $\mathbf{h}'_s$.

To illustrate, consider h'_{s1}.

$$\begin{aligned} h'_{s1} &= (\mu_{11} h_{s1} + \mu_{12} h_{s2} + \mu_{13} h_{s3}) \\ &= \frac{1}{8\pi\kappa} \left[\frac{\partial^2 I}{\partial q_1^2} (\mu_{22}\mu_{13} - \mu_{12}\mu_{32}) \right. \\ &\quad \left. + \frac{\partial^2 I}{\partial q_1 \partial q_2} (\mu_{11}\mu_{32} - \mu_{12}\mu_{13}) \right] . \end{aligned} \tag{A5}$$

The products of $\overline{\overline{\mu}}$ matrix elements above are recognized as proportional to the 13 and 23 cofactors of the $\overline{\overline{\mu}}^{-1}$ or $\overline{\overline{m}}$ matrix. Thus

$$h'_{s1} = \frac{-1}{8\pi\kappa} \frac{\partial}{\partial q_1} \left[\frac{\partial I}{\partial q_1} m_{13} + \frac{\partial I}{\partial q_2} m_{23} \right] \tag{A6}$$

h'_{s2} has a similar form so that the two transverse fields may be combined into a single gradient correction term. However h'_{s3} is quite different. After procedures similar to those outlined above one finds

$$\begin{aligned} h'_{s3} &= \frac{1}{8\pi\kappa} \left[\frac{\partial^2 I}{\partial q_1^2} m_{11} + \frac{\partial^2 I}{\partial q_2^2} m_{22} + 2 \frac{\partial^2 I}{\partial q_1 \partial q_2} m_{12} \right] \\ &= \frac{1}{8\pi\kappa} \nabla_q \cdot \overline{\overline{m}} \cdot \nabla_q I = \frac{1}{8\pi\kappa} \nabla^2 I = -\frac{1}{2\kappa} |\psi_0|^2 . \end{aligned} \tag{A7}$$

In the last form we have reverted to real space again and applied (35) of the text. Combining all three components we may summarize the results in vector form as Eq. (33).

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