# Structure of an isolated vortex in an anisotropic type-II superconductor

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The Ginzburg-Landau equations with general effective-mass anisotropy are diagonalized for a general direction  $\mathbf{v}$  of an isolated vortex core. For  $\mathbf{v}$  not parallel to one of the three crystal axis directions, the local magnetic induction  $\mathbf{b}$  contains components  $b_{\rho}$  and  $b_{\phi}$ , perpendicular to  $\mathbf{v}$ , which vanish as  $\rho^2$  away from the center of the core with coefficients that are odd in the azimuthal angle  $\phi$ . In the London limit far from the core,  $b_{\rho}$  and  $b_{\phi}$  are comparable to  $b_3 = \hat{\mathbf{v}} \cdot \mathbf{b}$ , and all fall off exponentially in  $\rho$ , with two distinct exponents, each of which depends explicitly upon the azimuthal angle  $\phi$  about  $\hat{\mathbf{v}}$ . The presence of  $b_{\rho}$  and  $b_{\phi}$  reduces the energy cost of the locking of the core into the lattice but does not remove it entirely, as the leading correction to the line energy is proportional to the parameter  $\beta^2$  (rather than  $\beta$ ), where  $\beta$  is the parameter introduced previously by the author. With the use of an ansatz, an exact form for the field components and reduced order parameter f in the core region is obtained. The lines of constant  $b_3$  and  $|b_1|$  in the core region are found for arbitrary effective-mass anisotropy and  $\hat{\mathbf{v}}$ . These forms should be observable by scanning tunneling microscopy and by large-momentum-transfer neutron-scattering experiments for fields slightly greater than  $H_{c1}$ . In addition, the angular dependence of  $H_{c1}$  should exhibit a kink, as the vortex cores prefer to lie along one of the crystal symmetry directions.

## I. INTRODUCTION

The recent discovery<sup>1,2</sup> of superconductivity in layered materials with high transition temperature  $T_c$  has led to a revival of interest<sup>3-5</sup> in the phenomenology of superconductivity in highly anisotropic systems. Although there is still some dispute about the question of order-parameter anisotropy,<sup>6</sup> the preponderance of the evidence is presently consistent with *s*-wave superconductivity,<sup>7-9</sup> with a large effective-mass anisotropy. Although the question of intralayer effective-mass anisotropy in the superconducting state has not yet been resolved for all systems, there is evidence<sup>10</sup> that the normal-state properties in some materials exhibit some degree of intraplanar effective-mass anisotropy, as well as a large (uniaxial) effective-mass anisotropy between the directions parallel and perpendicular to the conducting planes.

To date, there have been a number of attempts to treat the behavior of a vortex at an arbitrary external field direction relative to the crystal axes. Kogan<sup>11</sup> investigated the asymptotic (London) regime far from the core, and solved this case in Fourier space. Klemm and Clem<sup>12</sup> (hereafter referred to as I) neglected the components of the local magnetic induction perpendicular to the core direction v, and transformed the Ginzburg-Landau free energy exactly, using an anisotropic scale transformation, a rotation, and an isotropic scale transformation. Kogan<sup>11</sup> showed that the components of  $b \perp v$  are nonnegligible, suggesting that the transformation procedure of I is not valid away from the upper critical field  $H_{c2}$  for an arbitrary v direction. Recently, we showed<sup>13</sup> (hereafter referred to as II) that application of the Klemm-Clem transformations to the Ginzburg-Landau (mean-field) equations leads to a component  $a_3$  of the vector potential parallel to v, which causes a near locking of the vortex core onto the lattice. In that treatment, the components

 $b_{\rho}$  and  $b_{\phi}$  of **b** $\perp$ **v** were neglected, as it was assumed for simplicity that the dominant contributions to the core energy arose from the variations of the reduced order parameter f and  $b_3 = \mathbf{b} \cdot \hat{\mathbf{v}}$ .

In this paper, we assume only that there exists a direction v along which the order parameter and magnetic induction b do not vary. In Sec. II, we apply the Klemm-Clem transformations to the mean-field Ginzburg-Landau equations in such a way that the scaletransformed axes  $\hat{\mathbf{e}}_{3}$  is rotated parallel to v, but do not neglect the resulting components of  $b \perp v$ . These fully general transformed equations depend upon three new parameters,  $\mu$ ,  $\nu$ , and  $\phi_2$ , as well as the parameters  $\alpha$  of I and  $\beta$  of II, all of which are functions of the direction cosines of v with the crystal axes. There are four transformed (coupled, nonlinear) Ginzburg-Landau equations describing the spatial variation of the reduced order parameter f and the three magnetic induction com-ponents  $b_3$ ,  $b_{\rho}$ , and  $b_{\phi}$  (in transformed polar coordinates), as well as the Maxwell equation  $\nabla \cdot \mathbf{b} = 0$  in those coordinates. In Sec. III, we analyze the behavior of the core region, and find the general form for  $f, b_3, b_0$ , and  $b_{\phi}$  as  $\rho \rightarrow 0$ . With the aid of an ansatz, the azimuthal dependence of those quantities in the core region is found exactly. In Sec. IV, we analyze the London regime  $\rho \rightarrow \infty$ . In Sec. V, we calculate the lower critical field  $H_{c1}$ for an arbitrary direction of v, and show that the cost in energy as v is rotated away from a crystal axis is proportional to  $\beta^2$  for small  $\beta$ . In Sec. VI, we present some concluding remarks.

# II. TRANSFORMATION OF THE ANISOTROPIC GINZBURG-LANDAU EQUATIONS

The starting point for this calculation is the anisotropic Ginzburg-Landau free energy for the superconducting

state, relative to the normal state [Eq. (8) of I], which in reduced units can be written as<sup>12,13</sup>

$$F_{S} - F_{N} = \int d\mathbf{r} \left[ -f^{2} + \frac{1}{2}f^{4} + \sum_{\mu} \frac{m}{m_{\mu}} \left[ \frac{1}{\kappa^{2}} (\partial_{\mu}f)^{2} + a_{\mu}^{2}f^{2} \right] + \mathbf{b}^{2} \right],$$
(1)

where  $m = (m_1, m_2, m_3)^{1/3}$  is the effective-mass geometric mean,  $\kappa = \lambda/\xi$  is the usual GL parameter,  $\mathbf{b} = \nabla \times \mathbf{a}$  is the local magnetic induction in terms of the gaugetransformed vector potential  $\mathbf{a}, f = |\Psi/\Psi_0|$  is the relative magnitude of the local order parameter,  $m_{\mu}$  is the effective mass in the  $\mu = 1, 2, 3$  direction, and  $\partial_{\mu} \equiv \partial/\partial x_{\mu}$ . This notation is precisely the same as in II. In I, we found that this free energy could be transformed, assuming the direction of  $\mathbf{b}$  to be a constant. In II, we transformed the mean-field anisotropic GL equations, obtaining

$$\sum_{\mu} \frac{m}{m_{\mu}} \left[ -\frac{1}{\kappa^2} \partial_{\mu}^2 f + a_{\mu}^2 f \right] = f(1-f^2)$$
(2a)

and

$$\frac{-m}{m_{\mu}}a_{\mu}f^{2} = \nabla \times (\nabla \times \mathbf{a}) \cdot \hat{\mathbf{e}}_{\mu} = \sum_{\nu} \partial_{\nu}(\partial_{\mu}a_{\nu} - \partial_{\nu}a_{\mu}) , \quad (2b)$$

where  $\hat{\mathbf{e}}_{\mu} = \hat{\mathbf{x}}_{\mu}$  is a unit vector in the  $\mu = 1, 2, 3$  direction of the crystal. In both I and II, the direction of **b** was assumed constant, but in this treatment, we relax that restriction, assuming only that there is a direction **v** given by

$$\hat{\mathbf{v}} \equiv (\sin\theta_0 \cos\phi_0, \sin\theta_0 \sin\phi_0, \cos\theta_0) , \qquad (3)$$

along which the quantities f and **b** do not vary. This direction corresponds to the direction of the center of the vortex core, which is assumed to be a constant in the bulk sample. We neglect cases in which the center of the vortex core can bend, as this would require a local, rather than a global transformation procedure. In addition, as we shall see, the vortex cores prefer to lie along one of the crystal symmetry directions, so that bending of the core centers costs additional energy. Although such bending would be expected in a finite sample of nonellipsoidal shape, it is not expected to be important in a bulk sample, or a finite sample of ellipsoidal shape, which are the cases of interest here.

We now employ the transformations of I as in II, with the interpretation that the direction  $\hat{\mathbf{e}}_3 = \hat{\mathbf{v}}$ . As in I and II, we write

$$x_{\mu} = \frac{1}{\alpha} \left[ \frac{m}{m_{\mu}} \right]^{1/2} \sum_{\nu} \lambda_{\nu \mu} \tilde{x}_{\mu} , \qquad (4a)$$

$$\partial_{\mu} = \alpha \left[ \frac{m_{\mu}}{m} \right]^{1/2} \sum_{\nu} \lambda_{\nu \mu} \tilde{\partial}_{\nu} , \qquad (4b)$$

$$b_{\mu} = \alpha \left[ \frac{m}{m_{\mu}} \right]^{1/2} \sum_{\nu} \lambda_{\nu \mu} \tilde{b}_{\nu} , \qquad (4c)$$

and

$$a_{\mu} = \left(\frac{m_{\mu}}{m}\right)^{1/2} \sum_{nu} \lambda_{\nu\mu} \tilde{a}_{\nu} , \qquad (4d)$$

where

$$\boldsymbol{\alpha}(\boldsymbol{\theta}_{0},\boldsymbol{\phi}_{0}) \equiv \left[\sum_{v} \frac{m_{\mu}}{m} (\hat{\boldsymbol{e}}_{\mu} \cdot \hat{\boldsymbol{v}})^{2}\right]^{1/2}$$
(5)

is the anisotropy factor associated with the upper critical field  $H_{c2}$ . Note that at  $H_{c2}$ ,  $\hat{\mathbf{b}} = \hat{\mathbf{v}}$ , so this definition of  $\alpha$  is the same as in I and II in that limit. As in I and II, the rotation matrix  $\lambda_{\mu\nu}$  is given by [Eq. (4) of II]

$$\lambda_{\mu\nu} = \begin{bmatrix} \sin\phi' & -\cos\phi' & 0\\ \cos\theta'\cos\phi' & \cos\theta'\sin\phi' & -\sin\theta'\\ \sin\theta'\cos\phi' & \sin\theta'\sin\phi' & \cos\theta' \end{bmatrix}, \quad (6)$$

where  $\theta', \phi'$  are the angles the scale-transformed coordinates make with the original lattice,

$$\hat{e}' = (\sin\theta'\cos\phi', \sin\theta'\sin\phi', \cos\theta') , \qquad (7)$$

which are related (as in I and II) to the direction cosines of  $\hat{\mathbf{v}}$  by [Eq. (5) of II, with the replacement  $\hat{\mathbf{b}} \rightarrow \hat{\mathbf{v}}$ ]

$$\widehat{\mathbf{e}}' \cdot \widehat{\mathbf{e}}_{\mu} = \frac{1}{\alpha} \left[ \frac{m_{\mu}}{m} \right]^{1/2} \widehat{\mathbf{v}} \cdot \widehat{\mathbf{e}}_{\mu} . \tag{8}$$

As in I and II, transformation of the order-parameter equation [Eq. (2a)] leads to

$$-\frac{1}{\tilde{\kappa}^2}\tilde{\nabla}^2 + \tilde{a}^2 f = f(1-f^2) , \qquad (9)$$

where  $\tilde{\kappa} \equiv \kappa / \alpha$  and  $\alpha$  is given by Eq. (5). As in II, transformation of Eq. (2b) leads after multiplication by  $\lambda_{\gamma\mu}(m_{\mu}/m)$  and summation over  $\mu$  to

$$-\tilde{\alpha}_{\gamma}f^{2} = \alpha^{2} \sum_{\nu'\lambda\lambda'} (\Gamma_{\gamma\lambda'}\Gamma_{\lambda\nu'} - \Gamma_{\gamma\nu'}\Gamma_{\lambda\lambda'}) \tilde{\partial}_{\lambda}\tilde{\partial}_{\lambda'}\tilde{a}_{\nu'} , \quad (10)$$

where

$$\Gamma_{\alpha\beta} = \sum_{\nu} \frac{m_{\nu}}{m} \lambda_{\alpha\nu} \lambda_{\beta\nu} = \Gamma_{\beta\alpha} .$$
(11)

As in II, we now explicitly evaluate Eq. (10), but we now keep *all* of the components of  $\tilde{\mathbf{b}}$ , assuming only that

$$\tilde{\partial}_3 f = \tilde{\partial}_3 \tilde{a}_\mu = 0 . \tag{12}$$

We find

$$\tilde{a}_1 f^2 = -\tilde{\partial}_2 (\tilde{b}_3 + \epsilon_2 \tilde{b}_1 - \epsilon_1 \tilde{b}_2) , \qquad (13a)$$

$$\widetilde{a}_2 f^2 = \widetilde{\partial}_1 (b_3 + \epsilon_2 \widetilde{b}_1 - \epsilon_1 \widetilde{b}_2) , \qquad (13b)$$

and

$$\tilde{a}_{3}f^{2} = \epsilon_{1}\tilde{\partial}_{1}\tilde{b}_{3} + \epsilon_{2}\tilde{\partial}_{2}\tilde{b}_{3} + \epsilon_{3}\tilde{\partial}_{2}\tilde{b}_{1} - \epsilon_{4}\tilde{\partial}_{1}\tilde{b}_{2} + \epsilon_{5}(\tilde{\partial}_{1}b_{1} - \tilde{\partial}_{2}\tilde{b}_{2}) , \qquad (13c)$$

where

$$\boldsymbol{\epsilon}_1 \equiv \boldsymbol{\alpha}^2 (\Gamma_{32} \Gamma_{11} - \Gamma_{31} \Gamma_{12}) , \qquad (14a)$$

$$\epsilon_2 \equiv \alpha^2 (\Gamma_{32} \Gamma_{21} - \Gamma_{31} \Gamma_{22}) , \qquad (14b)$$

$$\epsilon_3 \equiv \alpha^2 (\Gamma_{22} \Gamma_{33} - \Gamma_{23}^2) , \qquad (14c)$$

$$\epsilon_4 \equiv \alpha^2 (\Gamma_{11} \Gamma_{33} - \Gamma_{13}^2) , \qquad (14d)$$

and

$$\epsilon_5 \equiv \alpha^2 (\Gamma_{33} \Gamma_{12} - \Gamma_{23} \Gamma_{13}) . \tag{14e}$$

The  $\epsilon_i$  may be explicitly evaluated by using Eqs. (6) and (11). We define

$$\bar{\alpha}(\phi_0) \equiv \alpha(\pi/2, \phi_0) = \left[\frac{m_1}{m} \cos^2 \phi_0 + \frac{m_2}{m} \sin^2 \phi_0\right]^{1/2} .$$
 (15)

The  $\epsilon_i$  are then given by

$$\epsilon_1 = \left(\frac{m_3}{m}\right)^{1/2} \sin(2\theta_0) \left(\frac{(m/m_3)[\overline{\alpha}(\phi_0)]^2 - 1}{2\overline{\alpha}(\phi_0)}\right), \quad (16a)$$

$$\epsilon_2 = \frac{(m_3/m)^{1/2} [(m_2 - m_1)/m] \alpha \sin \theta_0 \sin(2\phi_0)}{2\overline{\alpha}(\phi_0)} , \quad (16b)$$

$$\epsilon_{3} = \frac{\alpha^{2}(m_{3}/m)[(m_{1}/m)^{2}\cos^{2}\phi_{0} + (m_{2}/m)^{2}\sin^{2}\phi_{0}]}{[\bar{\alpha}(\phi_{0})]^{2}}$$

$$\epsilon_4 = \frac{(m_3/m)\cos^2\theta_0 + (m/m_3)\sin^2\theta_0[\overline{\alpha}(\phi_0)]^4}{[\overline{\alpha}(\phi_0)]^2} , \qquad (16d)$$

and

$$\epsilon_{5} = \frac{(m_{3}/m)[(m_{1}-m_{2})/m]\alpha\cos\theta_{0}\sin(2\phi_{0})}{2[\bar{\alpha}(\phi_{0})]^{2}} .$$
 (16e)

The expressions for  $\epsilon_1$  and  $\epsilon_2$  are identical to Eqs. (12a) and (12b) of II, with the interpretation that  $\theta_0$  and  $\phi_0$  are defined by the direction cosines of  $\hat{\mathbf{v}}$ , not  $\hat{\mathbf{b}}$ . Note that for uniaxial anisotropy  $(m_1 = m_2)$  both  $\epsilon_2$  and  $\epsilon_5$  vanish identically.

Equations (9) and (13), together with

$$\tilde{b}_3 = \tilde{\partial}_1 \tilde{a}_2 - \tilde{\partial}_2 \tilde{a}_1 , \qquad (17a)$$

$$\tilde{b}_2 = -\tilde{\partial}_1 \tilde{a}_2 , \qquad (17b)$$

$$\tilde{b}_1 = \tilde{\partial}_2 \tilde{a}_3 , \qquad (17c)$$

and

$$\tilde{\partial}_1 \tilde{b}_1 + \tilde{\partial}_2 \tilde{b}_2 = 0 \tag{17d}$$

[which are just the three components of  $\tilde{\mathbf{b}} = \tilde{\nabla} \times \tilde{\mathbf{a}}$ , and the Maxwell equation  $\tilde{\nabla} \cdot \tilde{\mathbf{b}} = 0$ ], give a closed set of equations for the order parameter and the  $\tilde{\mathbf{b}}_{\mu}$ . As in II, it is convenient to transform to cylindrical coordinates, as we assumed there is no spatial variation of the physical quantities along the direction ( $\hat{\mathbf{e}}_3$ ) of  $\hat{\mathbf{v}}$ . We thus write

$$\tilde{\boldsymbol{b}}_{\phi} = \tilde{\mathbf{b}} \cdot \hat{\boldsymbol{\phi}} = \tilde{\boldsymbol{b}}_2 \cos \tilde{\boldsymbol{\phi}} - \tilde{\boldsymbol{b}}_1 \sin \tilde{\boldsymbol{\phi}} , \qquad (18a)$$

$$\tilde{b}_{\rho} = \tilde{\mathbf{b}} \cdot \hat{\vec{\rho}} = \tilde{b}_1 \cos \tilde{\phi} + \tilde{\mathbf{b}}_2 \sin \tilde{\phi} , \qquad (18b)$$

and

$$\widetilde{b}_3 = \widetilde{\mathbf{b}} \cdot \widehat{\mathbf{v}}$$

The relevant Maxwell equation is, of course,

$$\frac{1}{\tilde{\rho}}\tilde{\partial}_{\rho}(\tilde{\rho}\tilde{b}_{\rho}) + \frac{1}{\tilde{\rho}}\tilde{\partial}_{\phi}\tilde{b}_{\phi} = 0 , \qquad (19)$$

where

$$\tilde{\partial}_{\rho} \equiv \frac{\partial}{\partial \tilde{\rho}}, \quad \tilde{\partial}_{\phi} \equiv \frac{\partial}{\partial \tilde{\phi}}$$

As in II, we define

$$\beta \equiv \frac{1}{2} (\epsilon_1^2 + \epsilon_2^2) \tag{20a}$$

and

$$\tan \bar{\phi}_0 = \frac{\epsilon_2}{\epsilon_1} , \qquad (20b)$$

and let  $\phi = \tilde{\phi} - \bar{\phi}_0$ . Similarly, we define

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$$\mu \equiv \frac{1}{2} (\epsilon_3 + \epsilon_4) , \qquad (21a)$$

$$v \equiv \frac{1}{2} [(\epsilon_3 - \epsilon_4)^2 + 4\epsilon_5^2]^{1/2}$$
, (21b)

$$\tan 2\phi_1 \equiv \frac{2\epsilon_5}{\epsilon_3 - \epsilon_4} , \qquad (21c)$$

and

$$\phi_2 \equiv \phi_1 + \overline{\phi}_0 \ . \tag{21d}$$

We now write

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$$\bar{b} \equiv \phi + \phi_2 = \tilde{\phi} + \phi_1 , \qquad (22a)$$

$$\tilde{\rho} = \rho$$
, (22b)

and

$$\tilde{b}_{\phi} = \sqrt{2\beta} b_{\phi} , \qquad (22c)$$

$$\widetilde{b}_{p} \equiv \sqrt{2\beta} b_{\rho} \quad , \tag{22d}$$

$$\widetilde{b}_3 \equiv b_3$$
, (22e)

for simplicity of notation, since it turns out that  $\bar{b}_{\phi}$  and  $\tilde{b}_{\rho}$  are both proportional to  $\sqrt{2\beta}$ , relative to  $\tilde{b}_3$  and f [that is, they vanish when  $\hat{\mathbf{v}}$  is directed along a crystal symmetry direction, for which  $\beta=0$ ]. For simplicity, we write

$$h(\rho,\phi) \equiv \cos\phi \,\partial_{\rho} b_{3} - \rho^{-1} \sin\phi \,\partial_{\phi} b_{3}$$
$$+ \mu [\rho^{-1} \partial_{\phi} b_{\rho} - \rho^{-1} \partial_{\rho} (\rho b_{\phi})]$$
$$+ \nu \cos(2\overline{\phi}) [\rho^{-1} \partial_{\phi} b_{\rho} + \rho \partial_{\rho} (b_{\phi} / \rho)]$$
$$+ \nu \sin(2\overline{\phi}) [\rho \partial_{\rho} (b_{\rho} / \rho) - \rho^{-1} \partial_{\phi} b_{\phi}] \qquad (23a)$$

and

$$g(\rho,\phi) \equiv b_3 - 2\beta(\cos\phi b_{\phi} + \sin\phi b_{\rho}) . \qquad (23b)$$

The Ginzburg-Landau equations for a vortex in a superconductor with general effective-mass anisotropy may now be written,

$$-\frac{1}{\tilde{\kappa}^{2}} \left[\rho^{-1} \partial_{\rho} (\rho \partial_{\rho} f) + \rho^{-2} \partial_{\phi}^{2} f\right] + f^{-3} \left[ (\partial_{\rho} g)^{2} + \rho^{-2} (\partial_{\phi} g)^{2} + 2\beta h^{2} \right] = f (1 - f^{2}) , \quad (24a)$$

$$b_{3} = \rho^{-1} \partial_{\rho} (\rho f^{-2} \partial_{\rho} g) + \rho^{-2} \partial_{\phi} (f^{-2} \partial_{\phi} g) , \qquad (24b)$$

$$b_{\phi} = -\partial_{\rho}(f^{-2}h) , \qquad (24c)$$

$$b_{\rho} = \rho^{-1} \partial_{\phi} (f^{-2} h) , \qquad (24d)$$

and we have the Maxwell equation,

$$\rho^{-1}[\partial_{\rho}(\rho b_{\rho}) + \partial_{\phi} b_{\phi}] = 0 , \qquad (24e)$$

where

$$\partial_{\rho} \equiv \partial/\partial_{\rho}, \quad \partial_{\phi} \equiv \partial/\partial_{\phi}, \quad \partial^2_{\phi} \equiv \partial^2/\partial\phi^2$$

Note that the variables  $\rho$ ,  $\phi$  are transformed variables, according to Eqs. (4a) and (22). In the case that  $b_{\phi}$  and  $b_{\rho}$ can be neglected, Eqs. (24a) and (24b) reduce to those [Eqs. (18) and (15)] of II. We remark that Eq. (24) contains the parameters  $\alpha$ ,  $\beta$ ,  $\mu$ ,  $\nu$ , and  $\phi_2$ . The quantity  $\overline{\phi}_0$  is present implicitly by Eq. (20b), but only serves to define the zero of the cylindrical coordinate system, as it does not enter explicitly into any of the equations. We note further that  $\alpha, \mu > 0$ , and  $\beta, \nu \ge 0$ .

The appropriate boundary conditions for the order parameter and magnetic induction must first be found before any calculations can be performed. From the flux quantization condition,

$$B = \frac{1}{S} \int_{S} \mathbf{b} \cdot d\boldsymbol{\sigma} = \frac{\Phi_{0}}{S} , \qquad (25a)$$

where  $\phi_0$  is the flux quantum, we obtain

$$\int_0^\infty \rho \, d\rho \int_0^{2\pi} d\phi \, b_3 = \frac{2\pi}{\tilde{\kappa}} \, . \tag{25b}$$

Using Eq. (24b), we obtain the boundary condition as  $\rho \rightarrow 0$ :

$$\int_{0}^{2\pi} \frac{d\phi}{2\pi} \frac{\rho}{f^2} \frac{\partial g}{\partial \rho} \bigg|_{\rho \to 0} = -\frac{1}{\tilde{\kappa}} , \qquad (26)$$

as we have assumed  $\rho(\partial g/\partial \rho) \rightarrow 0$  as  $\rho \rightarrow \infty$ . As  $\rho \rightarrow \infty$ , we expect  $f \rightarrow 1$ , and  $b_3, b_{\phi}, b_{\rho} \rightarrow 0$ ,  $\partial b_3/\partial \rho \rightarrow 0$ ,  $\partial b_{\phi}/\partial \rho \rightarrow 0$ ,  $\partial b_{\rho}/\partial \rho \rightarrow 0$ . We also assume  $f, b_3, b_{\phi}$ , and  $b_{\rho}$  are finite as  $\rho \rightarrow 0$ , and all quantities are periodic in  $\phi$ :  $f(\phi) = f(\phi + 2\pi), b_3(\phi) = b_3(\phi + 2\pi), b_{\rho}(\phi) = b_{\rho}(\phi + 2\pi)$ , and  $b_{\phi}(\phi) = b_{\phi}(\phi + 2\pi)$  for single valuedness.

## III. SOLUTION NEAR THE CENTER OF THE VORTEX CORE

We assume a trial solution of the form

$$f(\rho,\phi) = C_0(\phi)\rho - C_1(\phi)\rho^3 + C_2(\phi)\rho^5 - \cdots$$
, (27a)

$$b_3(\rho,\phi) = b_3(0) - a_0(\phi)\rho^2 + a_1(\phi)\rho^4 + \cdots$$
, (27b)

$$b_{\phi}(\rho,\phi) = e_0(\phi)\rho^2 - e_1(\phi)\rho^4 + \cdots$$
, (27c)

$$b_{\rho}(\rho,\phi) = d_0(\phi)\rho^2 - d_1(\phi)\rho^4 + \cdots$$
 (27d)

Equations (27c) and (27d) follow from Eqs. (24c) and (24d) and the finiteness assumption as  $\rho \rightarrow 0$ . Unlike the forms found in II, there are no logarithmic corrections (e.g.,  $\rho \ln \rho$ , etc. for f). The presence of  $b_{\rho}$  and  $b_{\phi}$  conspires to eliminate such terms exactly. Note that as  $\beta \rightarrow 0$ , the  $a_i$  and  $c_i$  reduce to constants. For arbitrary  $\beta$ , we then write

$$g(\rho,\phi) = b_3(0) - \zeta_0(\phi)\rho^2 + \zeta_1(\phi)\rho^4 - \cdots$$
 (28a)

and

$$h(\rho,\phi) = \chi_0(\phi)\rho^5 + \cdots, \qquad (28b)$$

where Eq. (28b) follows from Eqs. (27), (23a), (24c), and (24d), and the assumption that all quantities are finite as  $\rho \rightarrow 0$ . We can then expand Eqs. (24a) and (24b) in powers of  $\rho$ , solving for the various coefficients of each power. From Eq. (24b), the term of order  $\rho^{-2}$  gives

$$\frac{\partial}{\partial \phi} \left[ \frac{\zeta_0'(\phi)}{C_0^2(\phi)} \right] = 0 , \qquad (29)$$

which has the general solution  $\zeta_0' = \gamma C_0^2(\phi)$ , where  $\gamma$  is a constant. Since we require  $\zeta_0(\phi)$  to be periodic in  $\phi$ ,  $\zeta_0(\phi) = \zeta_0(\phi + 2\pi)$ , this would require  $C_0^2$  to be periodic in  $\phi$ , with no constant term unless  $\gamma = 0$ . Since for  $\beta = 0$ ,  $C_0$  is a constant, we are forced to accept the solution  $\gamma = 0$ , implying  $\zeta_0(\phi) = \zeta_0 = \text{const.}$ 

The terms of Eq. (24a) to order  $\rho^{-1}$  yield

$$-\frac{1}{\tilde{\kappa}^{2}} [C_{0}(\phi) + C_{0}^{\prime\prime}(\phi)] + \frac{4\zeta_{0}^{2}}{C_{0}^{3}(\phi)} = 0.$$
 (30)

Note that as  $\beta = 0$ , we expect  $C_{00}'' = 0$ ,  $\xi_{00} = C_{00}^2 / 2\tilde{\kappa}$ , as for the isotropic case, where the quantities  $F_{00} \equiv F_0(\beta=0)$ . For  $\beta \neq 0$ ,  $C_0(\phi)$  becomes  $\phi$  dependent. Equation (30) may be solved exactly for arbitrary  $\beta$ . We define

$$\overline{C}_0 = C_0(\phi) / C_{00} , \qquad (31)$$

$$\bar{\xi}_0 = \xi_0 / \xi_{00} ,$$
 (32)

relative to their respective  $\beta = 0$  values ( $C_{00}$  and  $\zeta_{00}$ , respectively). Multiplying Eq. (30) by  $\overline{C}'_{0}$ , and integrating, we have

$$\frac{1}{2}\overline{C}_{0}^{2} + \frac{1}{2}(\overline{C}_{0}')^{2} + \frac{1}{2}\frac{\overline{\zeta}_{0}^{2}}{\overline{C}_{0}^{2}} = \overline{E}_{0} , \qquad (33)$$

where  $\overline{E}_0$  is a constant of integration. Equation (33) describes the conservation of energy of the vortex core, and may be solved in a number of ways. By solving for  $\overline{C}_0$  in terms of  $\overline{C}_0$ , we may integrate directly to obtain

$$\overline{C}_{0}(\phi) = [\overline{E}_{0} + (\overline{E}_{0}^{2} - \overline{\zeta}_{0}^{2})^{1/2} \cos 2(\phi - \phi_{c})]^{1/2}, \qquad (34)$$

where  $\phi_c$  is a second constant of integration. Note that there is no solution for  $\overline{E}_0 < \overline{\zeta}_0$ , and that  $\overline{E}_0 > 0$  from Eq. (33). Hence, the only case in which  $\overline{C}_0$  could vanish for some angle would be for  $\zeta_0=0$ , which is certainly not the case as  $\beta \rightarrow 0$ . This result is therefore consistent with our assumption  $\zeta_0=$  const. We have investigated solving Eq. (30) with  $\zeta'_0=\gamma C_0^2$  for  $\gamma \neq 0$ , assuming perturbation theory in  $\gamma$ . Using Eq. (34) as the starting point ( $\gamma = 0$ ), it is not possible to obtain a  $\zeta_0(\phi)$  that is periodic in  $\phi$  for  $\gamma \neq 0$ . Hence, the assumption  $\gamma = 0$  is further supported.

Note that as  $\beta \rightarrow 0$ ,  $\overline{E}_0 = \overline{\zeta}_0 = 1$ , so that a perturbation series in powers of  $\beta$  should be possible for  $\overline{C}_0(\phi)$ . We write

$$\bar{E}_0 = 1 + \beta \bar{E}_{01} + \beta^2 \bar{E}_{02} + \cdots , \qquad (35a)$$

$$\overline{\zeta}_0 = 1 + \beta \overline{\zeta}_{01} + \beta^2 \overline{\zeta}_{02} + \cdots , \qquad (35b)$$

$$\overline{C}_0(\phi) = 1 + \beta \overline{C}_{01}(\phi) + \beta^2 \overline{C}_{02}(\phi) + \cdots$$
(35c)

We note that the normalization condition [Eq. (26)] is automatically satisfied to all orders in  $\beta$ , as is easily checked by substituting Eq. (34) into Eq. (26). It is easy to demonstrate that  $\overline{\xi}_{01} = \overline{E}_{01}$ , but  $\overline{E}_{02} > \overline{\xi}_{02}$  cannot be found in this way. We find

$$\overline{C}_{01}(\phi) = \frac{1}{2} \{ \overline{\zeta}_{01} + [2(\overline{E}_{02} - \overline{\zeta}_{02})]^{1/2} \cos (\phi - \phi_c) \} .$$
(36)

Hence, a core energy of order  $\beta^2$  can give rise to an azimuthal dependence of  $\overline{C}_0$  of order  $\beta$ . One could formally carry out this procedure to higher order, but it is not useful, as one must first find  $\overline{E}_0$  in terms of  $\overline{\zeta}_0$  to order  $\beta^2$ and beyond. In what follows, we have succeeded in that task.

From the order- $\rho^2$  terms in Eqs. (23b), (28a), (27c), and (27d), we have

$$\zeta_0 = a_0(\phi) + 2\beta [e_0(\phi)\cos\phi + d_0(\phi)\sin\phi] . \qquad (37)$$

The functions  $e_0(\phi)$  and  $d_0(\phi)$  are found from the Maxwell equation [Eq. (24e)] to satisfy

$$d_0(\phi) = -\frac{1}{3}e'_0(\phi) , \qquad (38)$$

where  $e'_0(\phi) \equiv de_0(\phi)/d\phi$ .

We then write out Eq. (23a) to order  $\rho$ , and use Eq. (37) to eliminate  $a_0(\phi)$  in favor of the constant  $\zeta_0$ ,

$$-\eta(3e_0 + \frac{1}{3}e_0'') + \xi[(e_0 - \frac{1}{3}e_0'')\cos 2(\phi + \phi_3) - \frac{4}{3}e_0'\sin 2(\phi + \phi_3)] = 2\xi_0\cos\phi ,$$
(39a)

where

$$\eta \equiv \mu - \beta , \qquad (39b)$$

$$\xi = (\beta^2 + \nu^2 + 2\beta\nu\cos 2\phi_2)^{1/2} , \qquad (39c)$$

and

$$\tan 2\phi_3 \equiv \frac{v \sin 2\phi_2}{\beta + v \cos 2\phi_2} , \qquad (39d)$$

and we have used Eq. (38) to write  $d_0$  and  $d'_0$  in terms of  $e_0$  and  $e''_0$ , respectively. To simplify Eq. (39a), we write

$$e_0(\phi) \equiv [\eta + \xi \cos 2(\phi + \phi_3)] \widetilde{e}_0(\phi) . \tag{40}$$

After a bit of algebra, we obtain

$$[\eta + \xi \cos 2(\phi + \phi_3)]^2 \tilde{e}_{0}''(\phi) + \{[\eta + \xi \cos 2(\phi + \phi_3)]^2 + 8(\eta^2 - \xi^2)\} \tilde{e}_{0}(\phi) = -6\xi_0 \cos\phi .$$
(41)

A particular solution to Eq. (41) is easy to find,

$$\tilde{e}_0(\phi) = -\frac{3\xi_0 \cos\phi}{\eta^2 - \xi^2} , \qquad (42a)$$

$$e_0(\phi) = -\frac{3\xi_0 \cos\phi}{4(\eta^2 - \xi^2)} [\eta + \xi \cos 2(\phi + \phi_3)] .$$
 (42b)

The homogeneous solutions to Eq. (41) can be written as an infinite series in powers of  $\eta + \xi \cos 2(\phi + \phi_3)$ , which is described in detail in Appendix A. As we shall see below, we shall neglect the homogeneous solutions.

From Eqs. (37) and (38), we now may find the forms of  $d_0(\phi)$  and  $a_0(\phi)$ ,

$$d_{0}(\phi) = -\frac{\xi_{0}}{\eta^{2} - \xi^{2}} \{ \sin\phi [\eta + \xi \cos 2(\phi + \phi_{3})] + 2\xi \cos\phi \sin 2(\phi + \phi_{3}) \}$$
(43a)

and

$$a_{0}(\phi) = \zeta_{0} \left[ 1 + \frac{\beta}{2(\eta^{2} - \xi^{2})} \times [2\eta + \xi \cos 2\phi_{3} + \eta \cos 2\phi + 2\xi \cos 2(\phi + \phi_{3})] \right].$$
(43b)

Comparing Eq. (43) with Eq. (34), we see that  $a_0(\phi)$  may be written as

$$a_0(\phi) = \gamma_1 C_0^2(\phi) + \gamma_2$$
, (44a)

where  $\gamma_1$  and  $\gamma_2$  are constants. We note that for  $\beta = 0$ ,  $a_{00} = C_{00}^2 / 2\tilde{\kappa}$ , so that the spatial variation of the field component parallel to the vortex core in the core region is related to that of the order parameter. In Sec. V, we show that the dominant contribution to the core free energy is proportional to  $\tilde{E}_0 / \tilde{\zeta}_0$ . Minimization of this quantity for  $\gamma_2 \ge 0$  requires  $\gamma_2 = 0$ . We therefore make the ansatz

$$a_0(\phi) = \gamma_1 C_0^2(\phi)$$
 (44b)

Physically, the ansatz states that the spatial variation of  $b_3$  near the vortex core is proportional to  $f^2$ , just as in an isotropic system. This ansatz is very powerful. Not only does it enable us to determine the constant  $\phi_c$ , but it also enables us to obtain an expression relating  $\overline{E}_0$  and  $\overline{\xi}_0$ . Using the ansatz, we obtain

$$\tan 2\phi_c = -\frac{2\nu\sin 2\phi_2}{\mu + \beta + 2\nu\cos 2\phi_2} , \qquad (45a)$$

$$\gamma_1 = \frac{(A_1^2 - \beta^2 A_2^2 / 4)^{1/2}}{\mu^2 - \nu^2 - 2\beta(\mu + \nu \cos 2\phi_2)} , \qquad (45b)$$

and

$$\overline{E}_{0} = \overline{\zeta}_{0} \left[ 1 - \frac{\beta^{2} A_{2}^{2}}{4 A_{1}^{2}} \right]^{-1/2}, \qquad (45c)$$

where

$$A_1 = \mu^2 - \nu^2 - \beta(\mu + \frac{3}{2}\nu\cos 2\phi_2) - \beta^2/2$$
 (45d)

and

$$A_{2}^{2} = (\mu + \beta)^{2} + 4\nu^{2} + 4\nu(\mu + \beta)\cos 2\phi_{2} . \qquad (45e)$$

In the above equations, we have written  $\eta$ ,  $\xi$ , and  $\phi_3$  in terms of  $\mu$ ,  $\nu$ ,  $\beta$ , and  $\phi_2$ , using Eqs. (39b)–(39d).

We see immediately that  $\overline{E}_0/\overline{\zeta}_0 = 1 + O(\beta^2)$ , as our perturbation expansion required, and that  $\overline{E}_0 \ge \overline{\zeta}_0$ , the equality holding only at  $\beta = 0$ .

We remark that the forms [Eqs. (42b) and (43a)] of the field components perpendicular to  $\hat{\mathbf{v}}$  are odd in  $\phi \rightarrow \phi + \pi$ , as was found in the London regime by Kogan.<sup>11</sup> The form of  $b_3$  is even in  $\phi \rightarrow \phi + \pi$ , since  $b_3$  does not vanish at the vortex core, in contrast to  $b_{\rho}$  and  $b_{\phi}$ .

Although our ansatz has enabled us to find the ratio  $\overline{E}_0/\overline{\xi}_0$ , we are unable to use it to find  $\overline{\xi}_0$  explicitly. This can only be done by solving the full equations for all values of  $\rho$ , by matching the boundary conditions at  $\rho \rightarrow 0$ 

with those of  $\rho \rightarrow \infty$ . Unfortunately, this procedure in nontrivial, as we shall see in Sec. IV. Even for  $\beta = 0$ , the coefficient  $C_{00}$  must be found in this way, as was done for an isotropic superconductor by Hu.<sup>14</sup> Nevertheless, we shall see in Sec. V that the ratio  $\overline{E}_0/\zeta_0$  is important, as it enables us to calculate the dominant contribution to the lower critical field  $H_{cl}$ .

# **IV. SOLUTION IN THE LONDON REGIME**

As  $\rho \to \infty$ ,  $f \to 1$ , with corrections that are expected to behave exponentially in  $\rho$ . The magnetic field components then satisfy

$$b_3 = \rho^{-1} \partial_{\rho} (\rho \partial_{\rho} g) + \rho^{-2} \partial_{\phi}^2 g , \qquad (46a)$$

$$b_{\phi} = -\partial_{\rho}h$$
, (46b)

$$b_{\rho} = \rho^{-1} \partial_{\phi} h \quad , \tag{46c}$$

where g,h are given by Eq. (23). After solving for g,h, one then finds the leading correction to f (from unity) by inserting the forms of g,h into Eq. (24a). Although one desires g and h rather than the components of **b**, Eqs. (46) are easier to solve for the **b** components. We therefore use Eq. (23) to write Eq. (46) entirely in terms of  $b_3$ ,  $b_\rho$ , and  $b_{\phi}$ . We have

$$b_{3} = \rho^{-1} \partial_{\rho} (\rho \partial_{\rho} b_{3}) + \rho^{2} \partial_{\phi}^{2} b_{3} - 2\beta \{ \rho^{-1} \partial_{\rho} [\rho \partial_{\rho} (\cos\phi \ b_{\phi} + \sin\phi \ b_{\rho})] + \rho^{-2} \partial_{\phi}^{2} (\cos\phi \ b_{\phi} + \sin\phi \ b_{\rho}) \} , \qquad (47a)$$

$$b_{\phi} = -\partial_{\rho} \{ \mu [\rho^{-1} \partial_{\phi} b_{\rho} - \rho^{-1} \partial_{\rho} (\rho b_{\phi})] + v \cos(2\bar{\phi}) [\rho^{-1} \partial_{\phi} b_{\rho} + \rho \partial_{\rho} (b_{\phi} / \rho)]$$
  
+  $v \sin(2\bar{\phi}) [\rho \partial_{\rho} (b_{\rho} / \rho) - \rho^{-1} \partial_{\phi} b_{\phi}] \} - \partial_{\rho} (\cos\phi \partial_{\rho} b_{3} - \rho^{-1} \sin\phi \partial_{\phi} b_{3}) ,$  (47b)

and a similar equation for  $b_{\rho}$ . In Eq. (47a), we denote the terms involving  $b_3$  as the homogeneous part of the equation, and the rest of the equation is the inhomogeneous part. Conversely, the terms involving  $b_3$  in Eq. (47b) are the inhomogeneous terms, as  $b_{\phi}$  and  $b_{\rho}$  are related by Eq. (24e). We first examine the homogeneous terms. We have

$$b_{3h} = \rho^{-1} \partial_{\rho} (\rho \partial_{\rho} b_{3h}) + \rho^{-2} \partial_{\phi}^{2} b_{3h}$$
, (48a)

$$b_{\phi h} = -\partial_{\rho} h_h \quad , \tag{48b}$$

$$b_{\rho h} = \rho^{-1} \partial_{\phi} h_h , \qquad (48c)$$

where  $h_h$  is the part of h with  $b_3$  set equal to zero. Equation (48a) can readily be solved by the separation of variables, yielding

$$b_{3h}(\rho,\phi) = \sum_{m=0}^{\infty} A_m \cos(m\phi) K_m(\rho) , \qquad (49)$$

where  $K_m(z)$  is a standard Bessel function, and the  $A_m$  are arbitrary constants. In order to solve Eqs. (48b) and (48c), we assume a trial form for  $b_{\phi h}$  and  $b_{\rho h}$ . We write

$$b_{\phi h} \sim \frac{e_{\infty}(\phi)e^{-\frac{1}{0}\rho}}{\rho^{s}} , \qquad (50a)$$

$$b_{\rho h} \sim \frac{d_{\infty}(\phi)e^{-t_0\rho}}{\rho^s}$$
, (50b)

as  $\rho \rightarrow \infty$ , where  $t_0 = t_0(\phi)$ . Maxwell's equation requires

$$d_{\infty}(\phi) = -t_0' e_{\infty}(\phi) / t_0 .$$
<sup>(51)</sup>

Combining Eq. (51) with the homogeneous part of Eq. (47b) leads to the equation determining  $t_0(\phi)$ ,

$$\mu(t_0^2 + {t'_0}^2) - \nu \cos(2\overline{\phi})(t_0^2 - {t'_0}^2) + 2\nu t_0 t'_0 \sin 2\overline{\phi} = 1 .$$
 (52)  
Although one could immediately find a solution to Eq.

Although one could immediately find a solution to Eq. (52), to find additional solutions, it is useful to write

$$t_0(\phi) = (\mu + \nu \cos 2\bar{\phi})^{1/2} f_0(\phi) .$$
 (53)

We then obtain

$$(\mu^2 - \nu^2) f_0^2 + (\mu + \nu \cos 2\bar{\phi})^2 f_0^2 = 1 .$$
 (54)

One solution is immediately obvious: taking  $f'_0(\phi)=0$ , we obtain  $f_0 = (\mu^2 - \nu^2)^{-1/2}$ . To find the most general solution of Eq. (54), we note that both terms on the right-hand side are  $\ge 0$ , so that each must separately be  $\le 1$ . Hence, we can write  $f_0(\phi) = A_0 \cos[g_0(\phi)]$ . An additional solution satisfies

$$g'_{0}(\phi) = (\mu^{2} - \nu^{2})^{1/2} (\mu + \nu \cos 2\overline{\phi})^{-1}$$
, (55a)

which can be directly integrated to yield

$$f_0(\phi) = \frac{\cos(\phi - \delta\phi)}{[\mu + \nu\cos(2\bar{\phi})]^{1/2}[\mu + \nu\cos(2\delta\phi)]^{1/2}} .$$
 (55b)

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Hence, the solutions for  $t_0(\phi)$  are

$$t_{01}(\phi) = \left[\frac{\mu + \nu \cos 2\bar{\phi}}{\mu^2 - \nu^2}\right]^{1/2}$$
(56)

and

$$t_{02}(\phi) = \frac{\cos(\bar{\phi} - \delta\phi)}{\left[\mu + \nu \cos(2\delta\phi)\right]^{1/2}} .$$
 (57)

We can find the full form of the homogeneous solutions even under  $\phi \rightarrow \phi + \pi$  by assuming a form

$$b_{\phi h} = t_0(\phi) \overline{b} [t_0(\phi)\rho] , \qquad (58a)$$

$$b_{\rho h} = -t'_0(\phi) \tilde{b}[t_0(\phi)\rho] , \qquad (58b)$$

which satisfies the Maxwell equation exactly. It is readily found that the even solutions are

$$b_{\phi h1} = t_{01}(\phi) K_1(t_{01}(\phi)\rho) , \qquad (59a)$$

and

$$b_{\phi h2} = t_{02}(\phi) \exp[\pm t_{02}(\phi)\rho]$$
 (59b)

Although it is implicit in Eq. (59b) that one only takes the sign inside the square brackets so as to obtain exponential decay as  $\rho \rightarrow \infty$ , there exists an isolated value of  $\phi$  for which no decay exists. Although the coefficient of  $b_{\phi h2}$  would vanish as  $t_{02}(\phi) \rightarrow 0$ , the coefficient of  $b_{\rho h2}$  would not. Hence, we must eliminate the form  $t_{02}(\phi)$  for the exponent.

To obtain the homogeneous solution odd under  $\phi \rightarrow \phi + \pi$ , one has to use a different, but less elegant procedure.

We expand Eq. (50) out further,

$$b_{\phi h} = e_{\infty 0}(\phi) e^{-t_0(\phi)\rho} / \rho^s + e_{\infty 1}(\phi) e^{-t_0(\phi)\rho} / \rho^{s+1} + \cdots, \qquad (60a)$$

$$b_{\rho h} = d_{\infty 0}(\phi) e^{-t_0(\phi)\rho} / \rho^s + d_{\infty 1}(\phi) e^{-t_0(\phi)\rho} / \rho^{s+1} + \cdots$$
(60b)

Using Maxwell's equation, we obtain equations for the  $d_{\infty i}(\phi)$  in terms of the  $e_{\infty i}(\phi)$  [e.g., Eq. (51) for  $d_{\infty 0}$ ]. We then use the form of Eq. (60) to solve Eq. (47b), equating terms of like  $\rho$  dependence. The expansion [Eq. (60)] is solvable for  $s = \frac{1}{2}$ . Using the substitution

$$e_{\infty 0}(\phi) = f_0(\phi) / t_0^{1/2}(\phi)$$
, (61a)

we obtain an equation relating  $f_0$  and  $e_{\infty 1}(\phi)$ ,

$$(\mu + \nu \cos 2\bar{\phi})^2 f_0(\phi) + [(\mu + \nu \cos 2\bar{\phi})^2 - \frac{7}{4}(\mu^2 - \nu^2)] f_0(\phi) = -2e_{\infty 1}(\phi) t_0^{3/2}(\phi)(\mu^2 - \nu^2) .$$
(61b)

Note that if we choose  $f_0(\phi) = t_0(\phi)$ , we recover the (even) solution given by Eq. (59a), expanded to order  $e^{-t_0(\phi)\rho}/\rho^{3/2}$ . To obtain a solution odd under  $\phi \rightarrow \phi + \pi$ , we choose  $f_0(\phi) = \cos(\overline{\phi} - \delta\phi)$ , leading to

$$b_{\phi h3} = \cos(\bar{\phi} - \delta\phi) \left[ \frac{e^{-x}}{x^{1/2}} \left[ 1 + \frac{7}{8x} + \cdots \right] \right]$$
(62a)

and

$$b_{\rho h 3} = -\frac{\nu \sin 2\bar{\phi} \cos(\bar{\phi} - \delta\phi)}{\mu^2 - \nu^2} \times \left[ \frac{e^{-x}}{x^{1/2}} \{ 1 - x^{-1} [\frac{7}{8} + z(\phi)] \} \cdots \right], \quad (62b)$$

where  $x = t_0(\phi)\rho$  and

$$z(\phi) = \frac{\nu \sin(\bar{\phi} + \delta\phi) - \mu \sin(\bar{\phi} - \delta\phi)}{\nu \sin 2\bar{\phi} \cos(\bar{\phi} - \delta\phi)} .$$
 (62c)

We note that  $b_{\phi h3}$  appears to be of the form  $\cos(\bar{\phi} - \delta\phi)f(x)$ , but that  $b_{\rho h3}$  does not have such a simple form. Hence, a general solution is not expected to exhibit such simple behavior. We note that while other solutions to Eq. (61b) are possible, the solution given by Eq. (62) has the same symmetry as the particular core solution,  $b_{\phi h3}$  and  $b_{\rho h3}$  being odd under  $\phi \rightarrow \phi + \pi$ , and that the form  $\cos(\bar{\phi} - \delta\phi)f(t_{01}\rho)$  appears to be consistent with Eq. (42b) as  $\beta \rightarrow 0$ , provided that  $\delta\phi = \phi_2$ , assuming  $f(x) \rightarrow x^2$  as  $x \rightarrow 0$ . The important point to consider, though, is just that there exists a form for the homogene-

ous solutions for  $b_{\phi}$  and  $b_{\rho}$  in the London regime exhibiting a  $\phi$  dependence of the exponential decay of the form  $t_{01}(\phi)$ , that cannot be ruled out on symmetry grounds. This point is the basis for the following approach for the general solution in the London regime.

As  $\beta \rightarrow 0$ , Eq. (47a) for  $b_3$  reduces to the homogeneous solution, which behaves as  $e^{-\rho}/\rho^{1/2}$  as  $\rho \rightarrow \infty$  from Eq. (49). However, to order  $\beta$ , the inhomogeneous terms for  $b_3$  behave as  $e^{-t_{01}(\phi)\rho}/\rho^{1/2}$ . Similarly, the particular solution for  $b_{\phi}$  behaves as  $\cos\phi e^{-\rho}/\rho^{1/2}$  from Eq. (47b), which competes with the homogeneous solution of the form  $e_{\infty 0}(\phi)e^{-t_{01}(\phi)\rho}/\rho^{1/2}$ . If we attempt a perturbation expansion in powers of  $\beta$ , it is necessary to perform the perturbation in the exponents. As  $\beta$  increases, the exponent characterizing the decay of  $b_3$  decreases and becomes  $\phi$  dependent. The exponent for  $b_{\phi}$  is also modified, and these two equations [Eqs. (47)] plus the analogous one for  $b_{\rho}$  must be solved self-consistently. This is only possible if  $b_3$ ,  $b_{\rho}$ , and  $b_{\phi}$  all have the same exponent, which is  $\phi$  dependent, unless  $\beta=0$ . We therefore assume that the general asymptotic forms for the field components as  $\rho \rightarrow \infty$  are

$$b_3 \sim a_{\infty}(\phi) e^{-t(\phi)\rho} / \rho^{1/2}$$
, (63a)

$$b_{\phi} \sim e_{\infty}(\phi) e^{-t(\phi)\rho} / \rho^{1/2}$$
, (63b)

$$b_{\rho} \sim d_{\infty}(\phi) e^{-t(\phi)\rho} / \rho^{1/2}$$
 (63c)

Using these asymptotic forms in Eq. (47), we obtain an equation for  $t(\phi)$ ,

$$[1 - (t^{2} - t'^{2})][1 - \mu(t^{2} - t'^{2}) + \nu \cos 2\bar{\phi}(t^{2} - t'^{2}) - 2\nu tt' \sin 2\bar{\phi}] = \beta(t^{2} + t'^{2})[t^{2} + t'^{2} + \cos 2\phi(t^{2} - t'^{2}) - 2tt' \sin 2\phi].$$
(64)

We note that as  $\beta \to 0$ , there are two solutions for t as we expect, given by setting each of the quantities in square brackets on the left side equal to zero. Thus, we recover the  $\beta=0$  solutions  $t \to 1, t_{01}(\phi)$ . It is possible to find perturbation forms for t for small  $\beta$  by expanding about these values. We find

$$t = \begin{cases} 1 - \frac{\beta \cos^2 \phi}{(1 - \mu + \nu \cos 2\bar{\phi})} + O(\beta^2) \\ t_{01}(\phi) - \frac{\beta(\mu^2 + \nu^2 + 2\mu\nu \cos 2\bar{\phi})[\mu^2 \cos^2 \phi + \nu^2 \cos^2(\bar{\phi} + \phi_2) + 2\mu\nu(\cos^2 \bar{\phi} - \sin^2 \phi_2)]}{(\mu^2 - \nu^2)^2 t_{01}(\phi)[(\mu^2 - \nu^2)(\mu + \nu \cos 2\bar{\phi}) - (\mu^2 + \nu^2 + 2\mu\nu \cos 2\bar{\phi})]} + O(\beta^2). \end{cases}$$
(65)

We note that for all  $\theta_0, \phi_0$ , we have  $\mu > \nu$ , and  $\mu + \nu < 1$ , so that these expansions are valid for  $\beta >> 1$ . We remark that  $\beta \neq 0$  causes both unperturbed exponents to decrease, increasing the range of the magnetic field components from the core. At finite  $\beta$ , both exponents are assumed to be the same.

We have not been able to find an analytic form for  $t(\phi)$  valid to all orders in  $\beta$ .

#### **V. LOWER CRITICAL FIELD**

We now are in a position to calculate the line energy  $\varepsilon$ and therefore the lower critical field  $H_{c1}$ . The free energy given by Eq. (1) can be transformed by the same transformations used in Eq. (4), as was shown in I and II, yielding a line energy per unit length of the form

$$\varepsilon = \int_0^{2\pi} d\phi \int_0^\infty \rho \, d\rho [b_3^2 + 2\beta (b_\rho^2 + b_\phi^2) + \frac{1}{2}(1 - f^4)] \,. \tag{66}$$

As in II, we multiply Eq. (24b) by  $\partial_{\rho}b_3$ , Eq. (24a) by  $\partial_{\rho}f$ , and add them together. After some algebra and integration by parts, we find

$$\varepsilon = \varepsilon_{\rm reg} + \varepsilon_{\rm irreg}$$
, (67a)

where

$$\varepsilon_{\rm reg} = \int_0^{2\pi} d\phi \int_0^{\infty} \rho \, d\rho (1 - f^2) \tag{67b}$$

and

$$\varepsilon_{\rm irreg} = 3\beta \int_0^{2\pi} d\phi \int_0^\infty \rho \, d\rho \left[ b_\rho^2 + b_\phi^2 + 2\beta (\cos\phi \, b_\phi + \sin\phi \, b_\rho)^2 - \rho g \partial_\rho (\cos\phi \, b_\phi + \sin\phi \, b_\rho) - \rho h^2 f^{-3} \partial_\rho f \right] \,. \tag{67c}$$

In order to evaluate these integrals approximately, one must obtain asymptotic forms for the functions that are valid in the region  $\rho \ge 1/\tilde{\kappa}$ , and then match the boundary conditions as  $\rho \rightarrow 0$ . Hence, it is not correct merely to use the asymptotic forms found in Sec. IV, as they do not lead to the correct boundary conditions as  $\rho \rightarrow 0$ , and hence will be inaccurate in the region near the core, which dominates the line energy. In the usual procedure (14), one finds an approximate expression for  $1-f^2$ which incorporates the boundary conditions as  $\rho \rightarrow 0$ , as we did in II (neglecting  $b_{\phi}$  and  $b_{\rho}$ ). Using Eq. (24a) for  $1-f^2$ , we find that in the intermediate regime (which dominates the line energy), we have

$$1 - f^2 \approx \frac{\zeta_0^2}{\tilde{\kappa}^2 \bar{C}_0^4 \rho^2} , \qquad (68)$$

which arises from the  $(\partial_{\rho}g)^2 f^{-3}$  term in Eq. (24a), treated as  $(f^{-2}\partial_{\rho}g)^2 f$ , using the boundary condition [Eq. (26)]. Hence, the regular contribution to  $\varepsilon$  is

$$\varepsilon_{\rm reg} \simeq \frac{\ln \tilde{\kappa}}{\tilde{\kappa}^2} \int_0^{2\pi} d\phi \frac{\bar{\xi}_0^2}{\bar{C}_0^4} = \frac{2\pi \ln \tilde{\kappa}}{\bar{\kappa}^2} \frac{\bar{E}_0}{\bar{\xi}_0} .$$
(69)

As we noted in Sec. III, the line energy is proportional to  $\overline{E}_0/\overline{\zeta}_0$ , and hence it costs energy for the vortex to point away from a crystal symmetry direction. For small  $\beta$ , this cost in energy is proportional to  $\beta^2$ . In II, we found a cost in energy proportional to  $\beta$  by neglecting the  $b_{\rho}, b_{\phi}$  components. Hence, the presence of  $b_{\rho}$  and  $b_{\phi}$  reduces the cost in energy for the core, as well as restoring analytic behavior for the field components and order parameter as  $\rho \rightarrow 0$ .

We recall that in our ansatz relating  $a_0(\phi)$  to  $C_0^2(\phi)$ , the particular core solution allowed for an additional constant term  $\gamma_2$ . It is easy to show that Eq. (69b) is minimized for  $\gamma_2=0$ , provided that  $\gamma_2$  is taken to be  $\geq 0$ . Although it is formally possible to have  $\gamma_2 < 0$ , provided that  $\gamma_1$  is sufficiently large, we do not believe such a possibility to be physical, as  $\overline{E}_0/\overline{\zeta}_0$  would then not have a minimum.

In a similar fashion, one can show that the irregular contributions to the line energy are all of order  $\tilde{\kappa}^{-2}$ , implying that for  $\tilde{\kappa} \gg 1$ , the line energy is approximately given by Eq. (69b). We recall that  $\overline{E}_0/\overline{\xi}_0$  was found using our ansatz, and given by Eq. (45c). Hence, we have

$$H_{c1,\parallel} \simeq \frac{\ln \tilde{\kappa} \, \overline{E}_0}{2 \tilde{\kappa} \overline{\zeta}_0} ,$$
 (70a)

and the other components of  $H_{c1}$  are given in the usual way (I and II),

$$\mathbf{H}_{c1} = \widehat{\mathbf{v}} H_{c1,\parallel} + \widehat{\boldsymbol{\theta}}_0 \frac{\partial H_{c1,\parallel}}{\partial \theta_0} + \frac{\widehat{\boldsymbol{\phi}}_0}{\sin \theta_0} \frac{\partial H_{c1,\parallel}}{\partial \phi_0} .$$
(70b)

Equation (70) is easily derived for an arbitrary  $\hat{\mathbf{v}}$  direction, since the Gibbs free energy per unit volume contains the term  $-\mathbf{H}\cdot\mathbf{B}/4\pi$ , where  $\mathbf{B}=\langle \mathbf{b} \rangle$ . Note that the volume averages of  $b_{\phi}$  and  $b_{\rho}$  vanish, so that **B** is parallel to  $\hat{\mathbf{v}}$ .

We note that with the aid of the ansatz, it has been possible to solve for the leading term in the line energy exactly, provided  $\ln \tilde{\kappa} \gg 1$ . As indicated by Eq. (45), the analytic form for  $H_{c1}$  is rather complicated for arbitrary  $\theta_0, \phi_0$ , but well behaved. Since the  $\beta$  dependence of  $H_{c1,\parallel}$ is intermediate between that of I and II, we expect kinks in the angular dependence of  $H_{c1}$  that are present for large effective-mass anisotropy. These kinks are most pronounced for a large effective-mass anisotropy, but should be present for anisotropies as low as those reported<sup>15</sup> in YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7- $\delta$ </sub>. We note that for that material (with an intraplanar effective-mass anisotropy), the position ( $\theta_0$  value) of the kink in  $H_{c1}(\theta_0, \phi_0)$  will depend upon  $\phi_0$ .

#### VI. DISCUSSION AND CONCLUSIONS

We have shown that the transformations of I are fully general for a straight vortex core. They give rise to magnetic field components perpendicular to the core direction, which behave as  $\rho^2$  away from the core center. The presence of  $b_{\phi}$  and  $b_{\rho}$  for the core directed away from a crystal lattice direction lowers but does not eliminate the cost in energy for the core to lie away from those directions, and restores analytic behavior as  $\rho \rightarrow 0$  for the order parameter and all field components.

Using the ansatz that in the core region, the deviation of the component of the magnetic field  $b_3$  parallel to the core direction from its maximum value in the center of the core is proportional to the square of the order parameter, we were able to solve explicitly for the line energy of the vortex, and hence determine  $H_{c1}$  exactly, assuming  $\ln \tilde{\kappa} \gg 1$ .

In the London regime far from the core, the field components fall off exponentially, with an exponent that depends in a complicated fashion upon the azimuthal angle about the vortex direction, unless the vortex is directed parallel to a crystal axis direction. The perpendicular components  $b_{\rho}$  and  $b_{\phi}$  are proportional to  $\hat{\beta}^{1/2}$  in amplitude, and odd under  $\phi \rightarrow \phi + \pi$ . In the core region, their azimuthal dependencies have simple analytic forms, which were found explicitly. We note that as the azimuthal dependence of the field components and of the order parameter in the London region is somewhat different than in the core region, the cross-sectional shape of the vortex depends upon the radial distance  $\rho$  from the core, but always exhibits the same symmetry. The order parameter and  $b_3$  are even number  $\phi \rightarrow \phi + \pi$ , whereas  $b_{\rho}$ and  $b_{\phi}$  are odd. To illustrate the behavior in the core region, we have calculated the order parameter and perpendicular magnetic field components in the core in real space (untransformed coordinates). We define an orthonormal vector set

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$$\overline{\mathbf{x}} = \overline{\mathbf{x}}(\sin\phi_0, -\cos\phi_0, 0) , \qquad (71a)$$

$$\overline{\mathbf{y}} = \overline{\mathbf{y}}(\cos\theta_0 \cos\phi_0, \cos\theta_0 \sin\phi_0, -\sin\theta_0) , \qquad (71b)$$

$$\bar{\mathbf{z}} = \bar{\mathbf{z}} (\sin\theta_0 \cos\phi_0, \sin\theta_0 \sin\phi_0, \cos\theta_0) , \qquad (71c)$$

such that  $\overline{z}$  points along  $\hat{v}$ . By inverting the transformations [Eq. (4)], we obtain

$$\tilde{x}_1 = \frac{\alpha}{\bar{\alpha}(\phi_0)} \left[ \frac{m}{m_3} \right]^{1/2} \bar{x} , \qquad (72a)$$

$$\tilde{x}_2 = \left[\frac{m_3}{m}\right]^{1/2} \bar{\alpha}(\phi_0) \bar{y} , \qquad (72b)$$

and

$$\tilde{x}_3 = \alpha^2 \bar{z} . \tag{72c}$$

With this real-space notation, we have

$$f^2/(C_{00}^2\bar{\zeta}_0) = A'_1\bar{x}^2 + \cdots,$$
 (73a)

where

$$A_{1}^{\prime} = \left[\frac{\alpha}{\overline{\alpha}(\phi_{0})}\right]^{2} \frac{m}{m_{3}} \left\{\frac{\overline{E}_{0}}{\overline{\xi}_{0}} + \left[\left(\frac{\overline{E}_{0}}{\overline{\xi}_{0}}\right)^{2} - 1\right]^{1/2} \times \cos^{2}(\overline{\phi}_{0} + \phi_{c})\right\}, \qquad (73b)$$

$$B_{1} = \left(\frac{m_{3}}{m}\right) \overline{\alpha}^{2}(\phi_{0}) \left\{\frac{\overline{E}_{0}}{\overline{\zeta}_{0}} - \left[\left(\frac{\overline{E}_{0}}{\overline{\zeta}_{0}}\right)^{2} - 1\right]^{1/2} \times \cos^{2}(\overline{\phi}_{0} + \phi_{c})\right\}, \quad (73c)$$

$$C_1 = 2\alpha \left[ \left( \frac{\overline{E}_0}{\overline{\zeta}_0} \right)^2 - 1 \right]^{1/2} \sin 2(\overline{\phi}_0 + \phi_c) .$$
 (73d)

Hence, the lines of constant order parameter and, with our ansatz, constant  $b_3$  are given by setting the righthand side of Eq. (73a) equal to a constant. This resulting equation is obviously an ellipse in the plane perpendicular to  $\hat{\mathbf{v}}$ , which for the full anisotropy of three distinct effective masses is rotated from the  $\hat{\mathbf{x}}$ , and  $\hat{\mathbf{y}}$  axes by the angle  $\theta = \frac{1}{2} \tan^{-1} [C_1 / (B_1 - A'_1)]$ . In Figs. 1 and 2, the lines of constant f and  $\tilde{b}_3$  in the  $\bar{x}$ - $\bar{y}$  plane normal to  $\hat{v}$  are plotted for the case of the effective masses  $m_1, m_2$ , and  $m_3$  in the ratio 1:2:25. In each part of Fig. 1,  $\phi_0$  is held constant, and various curves for different  $\theta_0$  values are shown. In Fig. 2,  $\theta_0$  is held constant at 90° (normal to the large effective-mass direction), and  $\phi_0$  is varied. In all of these plots, the value of f (or  $\tilde{b}_3$ ) is held constant. In Fig. 1(a), the vortex lies in the y-z plane of the crystal. We see that as  $\phi_0$  is increases from 0°, the ellipsoidal lines of constant f first became less eccentric, shrinking in the  $\overline{y}$ direction, while expanding in the  $\bar{x}$  direction. As  $\theta_0$  is increased further from 0°, the eccentricity again increases, but the major axis is now in the  $\overline{\mathbf{x}}$  direction. In Fig. 1(b),  $\phi_0$  is 60°, and the behavior is similar to that of Fig. 1(a), except that the line of the major axis rotates to the left by





FIG. 1. Shown are plots of the lines of constant order parameter f (and also constant  $b_3$ ) in the plane normal to the vortex core direction  $\hat{\mathbf{v}}$ . The effective masses are in the ratio  $m_1:m_2:m_3$  as 1:2:25. In each figure,  $\phi_0$  is held constant, and the different curves are for various  $\phi_0$  and  $\theta_0$  values. (a)  $\phi_0 = 90^\circ$ , (b)  $\phi_0 = 60^\circ$ , (c)  $\phi_0 = 45^\circ$ , (d)  $\phi_0 = 30^\circ$ , (e)  $\phi_0 = 0^\circ$ .

90° during the process of shrinking and expanding, as  $\theta_0$  increases from 0° to 90°. Similar, but more pronounced behavior is seen in Fig. 1(c) for  $\phi_0 = 45^\circ$ .

In Fig. 1(d), a very interesting situation occurs at  $\phi_0 = 30^\circ$ . The core struggles to avoid the regions of large cost in energy. As  $\theta_0$  increases from 0°, the major axis rotates first to the right, and then switches to the left between  $\theta_0 = 60^\circ$  and 70°. In Fig. 1(e), for which the vortex lies in the x-z plane, the lines of constant f and  $b_3$  first becomes more [rather than less, as in Fig. 1(a)] eccentric, expanding in both  $\overline{\mathbf{x}}$  and  $\overline{\mathbf{y}}$  directions as  $\theta_0$  is increased from 0°. Beyond  $\theta_0 = 30^\circ$ , the minor axis shrinks, while the major axis expands greatly, until at approximately 49° the eccentricity diverges. Beyond the point, the vortex is not allowed. At approximately 76°, the vortex reappears, with its major axis in the same direction as before, but with decreased eccentricity. As  $\theta_0$  is increased to 90°, the eccentricity first decreases, and then increases along the  $\bar{\mathbf{x}}$ direction, similar to the behavior in Fig. 1(a).

In Fig. 2, the vortex is in the x-y plane, and is free to point in any direction. As  $\phi_0$  is increased from 0°, the only change in the lines of constant f and  $b_3$  is a minor decrease in the minor axis, with the major axis remaining constant.

In Fig. 3, the excess core energy  $\overline{E}_0/\overline{\zeta}_0$  is plotted for the same effective-mass values as in Figs. 1 and 2, as a function of  $\theta_0$  and  $\phi_0$ . Each curve corresponds to the  $\phi_0$ value indicated in the legend. We note that the excess core energy vanishes at the crystal symmetry direction  $\theta_0 = 0^\circ$ , and is exceedingly small for  $\theta_0 = 90^\circ$ , even for  $\phi_0 \neq 0^\circ$ , for which  $\beta \neq 0$ . This was evidenced by the ordinary behavior seen in Fig. 2. For  $\phi_0 > 40^\circ$ , there is a smooth peak in the excess core energy in the vicinity of  $\theta_0 = 78^\circ$ . As  $\phi_0$  is decreases from 40°, a sharp jump in the excess core energy at  $\theta_0 \le 60^\circ$  is apparent for  $\phi_0 = 30^\circ$ . As  $\phi_0$  is decreased further, the cost in energy of the core exhibits a large peak at  $\theta_0 = 60^\circ$  for  $\phi_0 = 25^\circ$ , and for smaller values of  $\phi_0$ , this peak diverges. Hence, the core is not allowed in this region. This behavior will be seen as a kink in the angular dependence of  $H_{c1}$  as was shown in I and II, but will be intermediate in magnitude between those



FIG. 2. Shown are lines of constant f and  $b_3$  in the plane normal to  $\hat{\mathbf{v}}$  for  $\theta_0$  for 90°, and several values of  $\phi_0$ .



FIG. 3. Shown is a plot of the excess core energy  $\overline{E}_0/\overline{\zeta}_0$ , for effective masses in the ratios indicated as a function of  $\theta_0$  for various values of  $\phi_0$ . The three curves that go off the figure are divergent.

predictions, due to the  $\beta^2$  dependence of the excess core energy for  $\hat{\mathbf{v}}$  directions near to the crystal axes.

To illustrate the magnitude of the components of **b** perpendicular to  $\hat{\mathbf{v}}$ , we have calculated the scalar quantity  $\tilde{b}_{1}^{2} = \tilde{b}_{\rho} + \tilde{b}_{\phi}^{2}$  in real space. In the plane perpendicular to  $\hat{\mathbf{v}}, \tilde{b}_{1}^{2}$  obeys the equation

$$\frac{\tilde{b}_{\perp}^{2}}{F} = A_{2+}\tilde{x}_{1}^{4} + A_{2-}\tilde{x}_{2}^{4} + C_{2}\tilde{x}_{1}^{2}\tilde{x}_{2}^{2} + D_{+}\tilde{x}_{1}\tilde{x}_{2}^{3} + D_{-}\tilde{x}_{1}^{3}\tilde{x}_{2},$$
(74a)

where

$$A_{2\pm} = \eta^{2} (40 \pm 32 \cos 2\bar{\phi}_{0}) + \xi^{2} [28 \pm 24 \cos 2\bar{\phi}_{0} + 12 \cos 4(\phi_{2} - \bar{\phi}_{0})] + \eta \xi [40 \cos 2\phi_{2} \pm 83 \cos 2(\phi_{2} - \bar{\phi}_{0}) + 24 \cos 2(\phi_{2} - 2\bar{\phi}_{0})], \qquad (74b)$$

$$C_{2} = 80\eta^{2} + \xi^{2} [56 - 24\cos 4(\phi_{2} - \bar{\phi}_{0})] + \eta \xi [80\cos 2\phi_{2} - 48\cos 2(\phi_{2} - \bar{\phi}_{0})], \qquad (74c)$$

$$D_{\pm} = 64\eta^{2} \sin 2\bar{\phi}_{0} \pm 48\xi^{2} \sin 4(\phi_{2} - \bar{\phi}_{0}) + \eta \xi [\pm 96 \sin 2(\phi_{2} - 2\bar{\phi}_{0}) - 126 \sin 2(\phi_{2} - \bar{\phi}_{0})] ,$$
(74d)

and

$$F = \frac{\beta \zeta_0^2}{64(\eta^2 - \xi^2)^2} , \qquad (74e)$$

where  $\tilde{x}_1$  and  $\tilde{x}_2$  are given by Eq. (72).

For uniaxial anisotropy, the terms odd in  $\bar{x}$  and  $\bar{y}$  drop out, leaving an elliptical-like form for the lines of constant  $\tilde{b}_1$ . For full anisotropy, this form is not preserved by a simple rotation about the  $\hat{v}$  axis, however, since  $D_+ \neq D_-$  and  $A_{2+} \neq A_{2-}$ .

8

6

Θ.

0

In Fig. 4, we have shown the lines of constant  $\tilde{b}_1$  in the plane normal to  $\hat{\mathbf{v}}$ , for various  $\theta_0$  and  $\phi_0$  directions. In Fig. 4(a), the vortex is in the *y*-*z* plane and  $\theta_0$  is varied. The effective masses are the same as in Figs. 1-3. We observe that the lines of constant  $\tilde{b}_1$  are rounded parallelograms. Since  $\tilde{b}_1$  vanishes along the crystal symmetry directions, those values ( $\theta^{\circ}$  and 90°) of  $\theta_0$  are curves of infinite major and minor axes. In this figure, as  $\theta_0$  is increased from 0°, the figure maintains its shape for  $\theta_0 \leq 40^{\circ}$ , but a shrinking of the minor axis is noticeable for  $\theta_0 = 60^{\circ}$ . The minor axis shrinks further for  $\theta_0 \leq 80^{\circ}$ , but then expands for  $\theta_0 > 80^{\circ}$ , as does the major axis.

In Fig. 4(b),  $\phi_0 = 60^\circ$ , and the parallelograms present in Fig. 4(a) are greatly distorted, as if they were subject to a strain. As  $\theta_0$  is increased from 0°, the lines of constant  $\tilde{b}_{\perp}$  become rather elliptical at  $\theta_0 = 20^\circ$  with a major axis that is rotated from the  $\bar{y}$  direction, but four rounded corners are evident at  $\theta_0 = 40^\circ$ , two of them developing along an axis that is not perpendicular to the major axis direction. As  $\theta_0$  is increased further, the lines of constant  $\tilde{b}_{\perp}$  become unstable along this direction, forming distorted hy-

perbolas. Past  $\theta_0 = 20^\circ$ , the  $\tilde{b}_{\perp} = \text{const}$  lines again stabilize into rounded parallelograms, with the major axis in the  $\bar{y}$ direction. Similar but distinct instabilities are evident for  $\theta_0$  between 10° and 80° at  $\phi_0 = 30^\circ$  in Fig. 4(c). In Fig. 4(d),  $\phi_0 = 0^\circ$ , and the behavior is similar to that of Fig. 4(a). The only difference is due to the infinite core energy for certain  $\theta_0$  values. In the region of infinite core energy, the lines of constant  $\tilde{b}_{\perp}$  shrink to the origin, as all of the magnetic field becomes normal to  $\hat{v}$ . Hence, curves for  $\theta_0$  between 49° and 76° are just points at the origin.

Using the ansatz that  $b_3$  is proportional to  $f^2$  in the core, we have been able to find an exact solution for the vortex core shape in real space. This solution, while analytic in form, contains many interesting features, some of which have been illustrated in the figures. We believe that such behavior should be observable in low field measurements on anisotropic materials such as  $YBa_2Cu_3O_{7-\delta}$ . For  $H \ge H_{c1}$ , the vortices will be spaced sufficiently far apart that the vortex-vortex interactions should not greatly affect the magnetic field distribution in the individual cores, so that our exact solution should be applicable. In this regime, one ought to be able to observe directly the spatial distribution of the individual

50

10.0

7.5



90

 $\Phi_0 =$ 

FIG. 4. Shown are plots of the lines of constant  $\tilde{b}_1$ , in the plane normal to  $\hat{\mathbf{v}}$ , for the effective masses in the ratio  $m_1:m_2:m_3$  as 1:2:25. In each plot  $\phi_0$  is the same, and the various curves are for different values of  $\phi_0$ . (a)  $\phi_0 = 90^\circ$ , (b)  $\phi_0 = 60^\circ$ , (c)  $\phi_0 = 30^\circ$ , (d)  $\phi_0 = 0^\circ$ .

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vortex cores by scanning tunneling microscopy. One could also observe the magnetic field distribution in the cores by large-momentum-transfer neutron-scattering diffraction, as the vortices will form a lattice at low temperatures. The advantage of the neutron-scattering technique is that it samples the region of the vortices within the bulk of the sample, where the boundary effects are less important. The disadvantages of this technique are that one requires a periodic vortex lattice with a large intervortex spacing, and that one must examine the largemomentum-transfer part of the scattering cross section. The scanning tunneling microscope, on the other hand, has been shown<sup>16</sup> to be capable of mapping out the structure of an individual vortex in the layered compound NbSe<sub>2</sub>, for the case of  $H \| \hat{c}$ . Hence, this technique could clearly be applied to that material for the field in an arbitrary direction. Note that in NbSe<sub>2</sub>, the effective-mass anisotropy is sufficient that a kink in the  $H_{c1}(\theta_0)$  has been observed experimentally.<sup>17</sup> This technique is particularly applicable to the high- $T_c$  materials, which are complicated by irreversibility and vortex pinning of an as yet not understood nature, as one can examine the structure of an individual vortex core.

We reiterate that the solution for the vortex structure we have found is fully arbitrary, appropriate for anisotropic superconductors with three distinct effective masses. It thus can be applied to all crystal structures, assuming only that the symmetry of the order parameter is described by two components.

Note added in proof. After this work was completed, we became aware of similar (unpublished) work by N. Schopohl and A. Baratoff, using a different ansatz.

## ACKNOWLEDGMENTS

The author would like to thank the Ames Laboratory for its hospitality. The Ames Laboratory is operated for the U.S. Department of Energy by Iowa State University under Contract No. W-7405-Eng-82. This investigation was supported by the Director for Energy Research, Office of Basic Energy Sciences.

### APPENDIX A

In this appendix, we derive the homogeneous solutions to Eq. (41) for  $\tilde{e}_0(\phi)$ . We let  $\tilde{\phi} = \phi + \phi_3$ . From Eq. (41),

the homogeneous form  $\tilde{e}_{0h}(\tilde{\phi})$  satisfies

$$\eta + \xi \cos 2\tilde{\phi})^2 \tilde{e}_{0h}^{\prime\prime} + \tilde{e}_{0h} [(\eta + \xi \cos 2\tilde{\phi})^2 + 8(\eta^2 - \xi^2)] = 0 .$$
(A1)

Since the coefficients of  $\tilde{e}_{0h}$  and  $\tilde{e}_{0h}''$  are both periodic in  $\tilde{\phi}$  with period  $\pi$  (rather than  $2\pi$ ), and  $\tilde{e}_0$  is periodic with period  $2\pi$ ,  $\tilde{e}_{0h}$  contains terms periodic both in  $\pi$  and in  $2\pi$ . That is, in an expansion in powers of  $\cos\phi$  or  $\sin\phi$ , there are both odd and even powers of those quantities. We thus write  $x = \eta + \xi \cos 2\phi$ ,

$$\tilde{e}_{0h1} = \cos \phi f_{+}(x) , \qquad (A2a)$$

$$\tilde{e}_{0h2} = \sin \tilde{\phi} f_{-}(x) , \qquad (A2b)$$

and

$$\tilde{e}_{0h3} = f_3(x) . \tag{A2c}$$

We also write

$$f_{\pm} = \sum_{n=-\infty}^{\infty} a_n^{\pm} x^{x+s}$$
 (A3a)

and

$$f_3 = \sum_{n=-\infty}^{\infty} b_n x^{n+s'}, \qquad (A3b)$$

where the negative powers are allowed since

$$0 < \eta - \xi \le x \le \eta + \xi . \tag{A4}$$

Using the above forms for the  $\tilde{e}_{0hi}$ , we find

$$x^{2}f_{\pm}''(x)[\xi^{2}-(x-\eta)^{2}]+x^{2}f_{\pm}'(x)[2(\eta-x)\pm\xi]$$
  
+2(\eta^{2}-\xi^{2})f\_{\pm}(x)=0, (A5a)

and

$$4x^{2}f_{3}''(x)[\xi^{2}-(x-\eta)^{2}]+4x^{2}(\eta-x)f_{3}'(x)$$
  
+f\_{3}(x)[x^{2}+8(\eta^{2}-\xi^{2})]=0. (A5b)

Using the power-series expansions [Eq. (A3)] for  $f_{\pm}$  and  $f_{3}$ , we find that the coefficients satisfy the recursion relations

$$a_n^{\pm}(\eta^2 - \xi^2)(n+s+1)(2-n-s) + (n+s-1)\{[2\eta(n+s-1)\pm\xi]a_{n-1}^{\pm} + (n+s-2)a_{n-2}^{\pm}\} = 0$$
(A6a)

and

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$$b_n(\eta^2 - \xi^2)(n+s'+1)(2-n-s') + (2n+2s'-3)[4\eta b_{n-1}(n+s'-1) - b_{n-2}(2n+2s'-5)] = 0.$$
 (A6b)

It is convenient to choose s = 1 and  $s' - \frac{1}{2}$ . We then find

$$a_0^{\pm} = 0$$
, (A7a)

$$b_n = 0$$
 for  $n \ge 1$ . (A7b)

The parameters  $b_0$  and  $b_{-1}$  are arbitrary, as are  $a_1^{\pm}$ ,  $a_{-1}$ , and  $a_{-2}^{\pm}$ . For n < -1, the parameters  $b_n$  are then given by Eq. (A6b) in terms of  $b_0$  and  $b_{-1}$ . For n > 1, the  $a_n^{\pm}$ are given by Eq. (A6a) in terms of  $a_1^{\pm}$ , and for n < -2, the parameters  $a_n^{\pm}$  are given by Eq. (A6a) in terms of  $a_{-1}^{\pm}$ and  $a_{-2}^{\pm}$ . We thus have

$$f_{\pm}(x) = \sum_{n=1}^{\infty} a_n^{\pm} x^{n+1} + \sum_{n=1}^{\infty} a_{-n}^{\pm} x^{-n+1}$$
(A8a)

and

$$f_3(x) = \sum_{n=0}^{\infty} b_n x^{-n+1/2}$$
 (A8b)

From Eq. (A2) and Eqs. (40), (37), and (38) of the text, we see by inspection that  $\tilde{e}_{0h3}$  leads to a component to the coefficient  $a_0(\phi)$  of the reduced order parameter f that is odd in  $\phi \rightarrow \phi + \pi$ . Hence, this term is unphysical, implying  $b_n = 0$  for all n. The homogeneous terms  $\tilde{e}_{0h1}$  and  $\tilde{e}_{0h2}$  have the same symmetry as the particular solution,

and cannot be neglected on symmetry grounds. However, as the coefficients  $a_n^{\pm}$  and  $a_{-n}^{\pm}$  are determined from  $a_1^{\pm}$ ,  $a_{-1}^{\pm}$ , and  $a_{-2}^{\pm}$ , it is clear that unless  $a_1^{\pm} = a_{-1}^{\pm} = a_{-2}^{\pm}$ ,  $a_0(\phi)$  will be an infinite series in powers of  $C_0^2(\phi)$ . The only solution compatible with our ansatz is the particular solution. Hence, we drop the homogeneous solutions.

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