Identification of nematic superconductivity from the upper critical field

Jörn W. F. Venderbos, Vladyslav Kozii, and Liang Fu
Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA
(Received 1 April 2016; revised manuscript received 15 August 2016; published 26 September 2016)

Recent nuclear magnetic resonance and specific heat measurements have provided concurring evidence of spontaneously broken rotational symmetry in the superconducting state of the doped topological insulator $Cu_xBi_2Se_3$. This suggests that the pairing symmetry corresponds to a two-dimensional representation of the D_{3d} crystal point group, and that $Cu_xBi_2Se_3$ is a nematic superconductor. In this paper, we present a comprehensive study of the upper critical field H_{c2} of nematic superconductors within Ginzburg-Landau (GL) theory. Contrary to typical GL theories which have an emergent U(1) rotational symmetry obscuring the discrete symmetry of the crystal, the theory of two-component superconductors in trigonal D_{3d} crystals reflects the true crystal rotation symmetry. This has direct implications for the upper critical field. First, H_{c2} of trigonal superconductors with D_{3d} symmetry exhibits a sixfold anisotropy in the basal plane. Second, when the degeneracy of the two components is lifted by, e.g., uniaxial strain, H_{c2} exhibits a twofold anisotropy with characteristic angle and temperature dependence. Our thorough study shows that measurement of the upper critical field is a direct method of detecting nematic superconductivity, which is directly applicable to recently-discovered trigonal superconductors $Cu_xBi_2Se_3$, $Sr_xBi_2Se_3$, $Nb_xBi_2Se_3$, and $Tl_xBi_2Te_3$.

DOI: 10.1103/PhysRevB.94.094522

I. INTRODUCTION

Unconventional superconductors can be defined by superconducting order parameters that transform nontrivially under crystal symmetries. For a given superconductor, possible unconventional order parameters are classified by nonidentity representations of the crystal point group. Such representations are either one dimensional or multidimensional, and this distinction defines two classes of unconventional superconductivity [1,2]. The first class is exemplified by d-wave superconductors in cuprates [3,4], while the second class is exemplified by the p-wave superconductivity in Sr_2RuO_4 [5], with two degenerate components (p_x, p_y) at the superconducting transition temperature. Superconducting states in the second class spontaneously break lattice or time-reversal symmetry [6], in addition to the U(1) gauge symmetry, leading to thermodynamic and transport properties not seen in single-component superconductors. The search for superconductors with multicomponent order parameters is therefore of great interest.

The doped topological insulator $Cu_xBi_2Se_3$, a superconductor with $T_c \sim 3.8$ K [7,8], has recently attracted a lot of attention as a promising candidate for unconventional superconductivity [9–19]. Fu and Berg proposed that it may have an odd-parity pairing symmetry resulting from interorbital pairing in a strongly spin-orbit-coupled normal state [9]. While previous surface-sensitive experiments [20,21] drew disparate conclusions regarding the nature of superconductivity in this material, direct tests of the pairing symmetry in the *bulk* of $Cu_xBi_2Se_3$ have been carried out only very recently. A nuclear magnetic resonance (NMR) measurement [22] found that despite the threefold rotational symmetry of the crystal, the Knight shift displays a twofold anisotropy below T_c as the field is rotated in the basal plane. The twofold anisotropy is also found in the specific heat of the superconducting state under magnetic fields down to $H = 0.03$ T corresponding to $H/H_{c2} \sim 0.015$ [23]. Both experiments found that the twofold anisotropy vanishes in the normal state, establishing that the superconducting state of $Cu_xBi_2Se_3$ spontaneously breaks the threefold rotational symmetry. This is only possible when the order parameter belongs to the two-dimensional E_u or E_g representation of the D_{3d} point group. The E_g pairing has been ruled out by comparing the theoretically expected gap structure [24] with specific heat data [8,23]. These results taken together strongly suggest that the pairing symmetry of $Cu_xBi_2Se_3$ is E_u, an odd-parity pairing with two-component order parameters [9].

Spontaneous rotational symmetry breaking due to superconductivity is a rare and remarkable phenomenon. Superconductors exhibiting rotational symmetry breaking from multicomponent order parameters can be called nematic superconductors [24], in analogy with the nematic liquid crystals and nematic electronic states in nonsuperconducting metals [25,26]. Nematic and chiral superconductivity, the latter breaking time-reversal symmetry, are the two distinct and competing states of multicomponent superconductors, corresponding to real and complex order parameters, respectively [1,6]. Broken rotational symmetry has previously been reported in the heavy-fermion superconductor UPt_3 [27] under a magnetic field [28]. In addition, the A phase in a narrow temperature range at zero field is likely rotational symmetry breaking, which, however, may be due to antiferromagnetic order already present in the normal state [29,30]. Thus the recent discovery of broken rotational symmetry in $Cu_xBi_2Se_3$, without broken time-reversal symmetry, may potentially open a fruitful research direction.

Motivated by the recent experimental progress, in this work we study the upper critical field H_{c2} of trigonal nematic superconductors within the framework of Ginzburg-Landau (GL) theory. Such GL theory admits a trigonal gradient term which is not allowed in hexagonal crystals [31]. We relate the gradient terms to Fermi surface and gap function anisotropies by a microscopic calculation of the GL coefficients. Building on and generalizing the previous work [31], we show that the upper critical field generically displays a sixfold anisotropy

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within the basal plane of trigonal crystals. We further show that a uniaxial strain acts as a symmetry-breaking field in nematic superconductors, which directly couples to the bilinear of the two-component superconducting order parameter. As a result, H_{c2} in the basal plane exhibits a twofold anisotropy with a distinctive angle and temperature dependence, similar to theoretically expected results for UPt_3 in the presence of antiferromagnetic order [32,33]. Our findings suggest that measurement of the upper critical field is a direct method of detecting nematic superconductivity. In particular, this method may shed light on the pairing symmetries of other superconducting doped topological insulators $Sr_xBi_2Se_3$ [34,35], $Nb_xBi_2Se_3$ [36], and $Tl_xBi_2Te_3$ [37], which have yet to be determined.

II. GINZBURG-LANDAU THEORY

We start by constructing the GL theory of odd-parity two-component superconductivity in crystals with D_{3d} point group and strong spin-orbit coupling. The pairing potential $\hat{\Delta}(\vec{k})$, which is a $\vec{k}$-dependent matrix in spin space, takes the following form

$$\hat{\Delta}(\vec{k}) = \eta_1 \hat{\Delta}_1(\vec{k}) + \eta_2 \hat{\Delta}_2(\vec{k}). \tag{1}$$

The pairing potential is a linear superposition of two degenerate components $\hat{\Delta}_{1,2}(\vec{k})$, the basis functions of the two-dimensional pairing channel E_u (specific gap functions are given in the Supplemental Material, Sec. III [47]). For odd-parity superconductors the pairing components satisfy $\hat{\Delta}_{1,2}(-\vec{k}) = -\hat{\Delta}_{1,2}(\vec{k})$. As basis functions of E_u, the two partners $\hat{\Delta}_{1,2}(\vec{k})$ transform differently under the mirror symmetry $x \to -x$, i.e., $\hat{\Delta}_1(\vec{k})$ is even whereas $\hat{\Delta}_2(\vec{k})$ is odd. A key property of (doped) Bi_2Se_3 materials is strong spin-orbit coupling that locks the electron spin to the lattice. The two complex fields $\eta_{1,2}$ define the superconducting order parameters $\eta = (\eta_1, \eta_2)^T$. In contrast, in the case of triplet superconductors in spin-rotation invariant materials the order parameter components are vectors in spin space.

The GL theory of two-component superconductivity is formulated in terms of the order parameters η, and the GL free energy $F_{\rm tot} = \int d^3\vec{x}\, f_{\rm tot}$ is the sum of a homogeneous term and a gradient term given by $f_{\rm tot} = f_{\rm hom} + f_D$, where $f_{\rm hom}$ and f_D are the corresponding free energy densities. In addition, the free energy contains a Maxwell term $f_{\rm EM} = (\vec{\partial} \times \vec{A})^2/8\pi$, which for our purposes can be taken as a constant. The free energy densities $f_{\rm hom}$ and f_D are polynomial expansions in the order parameter fields and their gradients and consist of all terms invariant under the symmetry group of the crystal. For two-component trigonal superconductors the homogeneous contribution is the same as the corresponding expression for hexagonal symmetry [1,6],

$$f_{\rm hom} = A\eta^\dagger\eta + B_1(\eta^\dagger\eta)^2 + B_2|\eta_1^*\eta_2 - \eta_2^*\eta_1|^2, \tag{2}$$

to fourth order in η, and we have defined $\eta^\dagger = (\eta_1^*, \eta_2^*)$. The coefficients $A \propto T - T_c$ and $B_{1,2}$ are phenomenological constants of the GL theory. The sign of GL coefficient B_2 determines the nature of the superconducting state, selecting either chiral or nematic order [24,38].

Spatial variation of the superconducting order parameter is captured by the gauge-invariant gradient $D_i = -i\partial_i - qA_i$, with $\vec{A}$ the electromagnetic vector potential and $q = -2e$. In case of multicomponent order parameters, there generally exist multiple independent gradient terms which are allowed by crystal symmetry. It is insightful to present all gradient terms in order of "emergent symmetry." For crystals with a principal rotation axis along the z direction, such as the three- and sixfold rotations of trigonal and hexagonal crystals, four gradient terms with full continuous in-plane rotational symmetry are present and given by [1,39,40]

$$\begin{aligned} f_D = {} & J_1(D_i\eta_a)^* D_i\eta_a + J_2\epsilon_{ij}\epsilon_{ab}(D_i\eta_a)^* D_j\eta_b \\ & + J_3(D_z\eta_a)^* D_z\eta_a + J_4[|D_x\eta_1|^2 + |D_y\eta_2|^2 \\ & - |D_x\eta_2|^2 - |D_y\eta_1|^2 + (D_x\eta_1)^* D_y\eta_2 + (D_y\eta_1)^* D_x\eta_2 \\ & + (D_x\eta_2)^* D_y\eta_1 + (D_y\eta_2)^* D_x\eta_1] \end{aligned} \tag{3}$$

(summation understood, $i = x, y$, $a = 1,2$), and $J_{1,2,3,4}$ are the phenomenological GL coefficients. The first three terms are invariant under independent U(1) rotation of coordinates and order parameters, and thus have an emergent U(1) × U(1) symmetry, whereas the gradient term with coefficient J_4 is invariant under arbitrary joint rotations of coordinates and order parameters, i.e., an emergent U(1) symmetry. Therefore, f_D does not reflect the discrete rotational symmetry of the crystal. However, a gradient term $f_{D,\rm trig}$, which we call trigonal gradient term, is uniquely present in crystals with trigonal symmetry, but not allowed in hexagonal crystals [31]. It is given by the expression

$$\begin{aligned} f_{D,\rm trig} = {} & J_5[(D_z\eta_1)^* D_x\eta_2 + (D_z\eta_2)^* D_x\eta_1 \\ & + (D_z\eta_1)^* D_y\eta_1 - (D_z\eta_2)^* D_y\eta_2 + \text{c.c.}]. \end{aligned} \tag{4}$$

The appearance of this gradient term, which has D_{3d} symmetry, can be understood from angular momentum, since in trigonal symmetry $L = 3$ is equivalent to $L = 0$. Indeed, in momentum space ($D_i \to q_i$) the trigonal gradient term can be expressed as $iq_z(q_-\eta_+^*\eta_- - q_+\eta_-^*\eta_+)$, where $q_\pm = q_x \pm iq_y$ and similarly for $\eta_{1,2}$. The relative phases between η_+ (q_+) and η_- (q_-) are determined by mirror symmetry: η_1 (η_2) is even (odd) under $x \to -x$. It follows from the structure of $f_{D,\rm trig}$ that the spatial variation of the order parameter in the basal plane is coupled to spatial variation in the z -direction, which is in sharp contrast to hexagonal and tetragonal crystals. In the rest of this paper we map out the consequences of trigonal crystal anisotropy in the GL theory for the upper critical field.

III. UPPER CRITICAL FIELD IN THE BASAL PLANE

The angular dependence of H_{c2} was first proposed as a method to establish the multicomponent nature of unconventional superconductors in the context of heavy-fermion superconductors [41–43]. The key idea is as follows. For the class of single-component (e.g., s-wave) superconductors with trigonal, tetragonal, and hexagonal symmetry, H_{c2} is always isotropic within the GL theory, due to the emergence of $U(1)$ rotational symmetry to second order in the gradients. In case of multicomponent superconductors, effects of crystal anisotropy can appear in the GL theory, removing the emergent U(1) symmetry, but this crucially depends on crystal symmetry.

For instance, hexagonal systems with multicomponent order parameters do not show in-plane H_{c2} anisotropy due to the emergent rotational symmetry of Eq. (3), whereas tetragonal symmetry can give rise to an angular dependence of H_{c2} with fourfold symmetry [42]. In trigonal crystals, H_{c2} can exhibit a sixfold anisotropy in the basal plane [31] as of Eq. (4). Here we map out the basal plane upper critical field of trigonal superconductors for general GL gradient coefficients.

Within GL theory, the upper critical field is calculated by solving the GL equations obtained from $F_{\rm tot}$, keeping only terms linear in η since the order parameter is small at H_{c2}. Therefore, the calculation also applies to chiral superconductors. The resulting system of GL equations, which is given by

$$\begin{aligned} -A\eta_a =\ & J_1(D_x^2+D_y^2)\eta_a + J_3 D_z^2\eta_a + J_2\epsilon_{ab}[D_x,D_y]\eta_b \\ & + J_4\big[(D_x^2-D_y^2)\tau^z_{ab} + \{D_x,D_y\}\tau^x_{ab}\big]\eta_b \\ & + J_5\big[\{D_z,D_x\}\tau^x_{ab} + \{D_z,D_y\}\tau^z_{ab}\big]\eta_b, \end{aligned} \tag{5}$$

can be solved as a two-component harmonic oscillator problem, leading to a Landau-level spectrum from which H_{c2} is determined as the lowest Landau-level solution. The coupling of the two harmonic oscillators is determined by the structure of the GL equations and is in general complicated by the presence of multiple gradient terms. In hexagonal and tetragonal systems, straightforward or even exact analytical expressions for H_{c2} can be found [42]. In contrast, the trigonal gradient term of Eq. (4) couples basal plane gradients to gradients in the orthogonal direction, giving rise to a different set of harmonic oscillator equations to which previous methods do not apply. A special limiting case was considered in Ref. [31]. We generalize this result by solving the GL equations in the presence of an in-plane magnetic field for general gradient coefficients. In deriving the general solution we adopt an operator based approach and exploit that harmonic oscillator mode operators corresponding to different cyclotron frequencies can be related by squeezing operators. Here we present and discuss the main results, and give a detailed account of the lengthy calculations in the Supplemental Material (SM) [47]. For convenience, below we will refer to the appropriate section of the SM.

To demonstrate the key features of H_{c2} in trigonal crystals, we will focus the discussion on the most physical case, where trigonal anisotropy effects may be considered weak and J_5 can be treated as perturbation. We take the magnetic field $\vec{H}$ in the basal plane to be given by $\vec{H} = H(\cos\theta, \sin\theta, 0)^T$, which corresponds to a vector potential $\vec{A} = Hz(\sin\theta, -\cos\theta, 0)^T$. It is convenient to rotate the basal plane GL gradients $D_{x,y} = -i\partial_{x,y} + 2eA_{x,y}$ according to the transformation

$$\begin{pmatrix} D_\parallel \\ D_\perp \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}\begin{pmatrix} D_x \\ D_y \end{pmatrix}, \tag{6}$$

such that $D_\parallel$ is along the field and $D_\perp$ is perpendicular to the field. These operators satisfy $[D_\parallel, D_\perp] = [D_\parallel, D_z] = 0$, and $D_\perp$ and D_z define the magnetic algebra $[D_z, D_\perp] = -2ieH$. Writing Eq. (5) in terms of $D_\perp$ and D_z, and setting $D_\parallel \eta_a = 0$ (i.e., no modulation along the field), one obtains

$$\begin{aligned} -A\eta_a =\ & \big(J_1 D_\perp^2 + J_3 D_z^2\big)\eta_a \\ & - J_4 D_\perp^2\big(\cos 2\theta\,\tau^z_{ab} + \sin 2\theta\,\tau^x_{ab}\big)\eta_b \\ & + J_5\{D_z, D_\perp\}\big(-\cos\theta\,\tau^z_{ab} + \sin\theta\,\tau^x_{ab}\big)\eta_b. \end{aligned} \tag{7}$$

Next, it is convenient to diagonalize the term proportional to J_4. This is achieved by a rotation of the order parameters given by

$$\begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} f_1 \\ f_2 \end{pmatrix}. \tag{8}$$

In terms of the rotated order parameters $(f_1, f_2)^T$ the GL equations read

$$\begin{aligned} & -A\begin{pmatrix} f_1 \\ f_2 \end{pmatrix} \\ & = \begin{pmatrix} J_3 D_z^2 + (J_1 - J_4)D_\perp^2 & 0 \\ 0 & J_3 D_z^2 + (J_1 + J_4)D_\perp^2 \end{pmatrix}\begin{pmatrix} f_1 \\ f_2 \end{pmatrix} \\ & \quad + J_5\{D_z, D_\perp\}\begin{pmatrix} -\cos 3\theta & \sin 3\theta \\ \sin 3\theta & \cos 3\theta \end{pmatrix}\begin{pmatrix} f_1 \\ f_2 \end{pmatrix}. \end{aligned} \tag{9}$$

Note that only the term proportional to J_5 depends on the angle θ. We now describe solutions to Eq. (9) obtained by treating J_5 as a perturbation.

To start, let us consider taking both $J_4 = J_5 = 0$. Solving the GL equations then yields two degenerate series of Landau levels with cyclotron frequency $\omega = \sqrt{J_1 J_3}$, with the upper critical field given by $H_{c2} = -A/2e\omega = -A/2e\sqrt{J_1 J_3}$ (more details are provided in Sec. II B of the SM [47]). Including the gradient contribution in Eq. (3) proportional to J_4 simply makes the cyclotron frequencies inequivalent, $\omega_{1,2} = \omega\sqrt{1 \mp |J_4|J_3/\omega^2} = \omega\sqrt{1 \mp |J_4|/J_1}$, and increases the upper critical field to $H_{c2} = -A/2e\omega_1$. This defines the exactly solvable unperturbed system. Then, introducing trigonal perturbation parametrized by J_5 couples the two series of Landau levels with different frequencies in a nontrivial way: The coupling of in-plane and out-of-plane gradients implies a coupling of canonically conjugate operators of the form $\{D_z, D_\perp\} \sim \{-i\partial_z, z\}$. To solve the system of GL equations we assume that crystal anisotropy effects are weak and use second order perturbation theory to obtain the correction to the cyclotron frequency $-\delta\omega_1$. (The calculations are lengthy and described in detail in Sec. II B 3 of the SM [47].) The upper critical field then becomes $H_{c2} = \widetilde{H}_{c2}(1 + \delta\omega_1/\omega_1)$ with $\widetilde{H}_{c2} \equiv -A/2e\omega_1$. We find H_{c2} to lowest order in J_5 as

$$\frac{H_{c2}(\theta)}{\widetilde{H}_{c2}} = 1 + \frac{J_5^2}{2\omega_+^2}\left[\frac{\cos^2 3\theta}{\left(1 - \frac{\omega_-}{\omega_+}\right)^2} + \frac{\sin^2 3\theta}{1 - \frac{\omega_-}{\omega_+}} F\left(\tfrac{\omega_-}{\omega_+}\right)\right], \tag{10}$$

where the frequencies $\omega_\pm$ are defined as $\omega_\pm = (\omega_2 \pm \omega_1)/2$. In the limit of small J_4/J_1 these frequencies become $\omega_+ \sim \omega$ and $\omega_- \sim \omega|J_4|/2J_1$. The function $F(x)$ arises due to the coupling of two series of Landau levels with different cyclotron frequencies and oscillator eigenfunctions. It takes

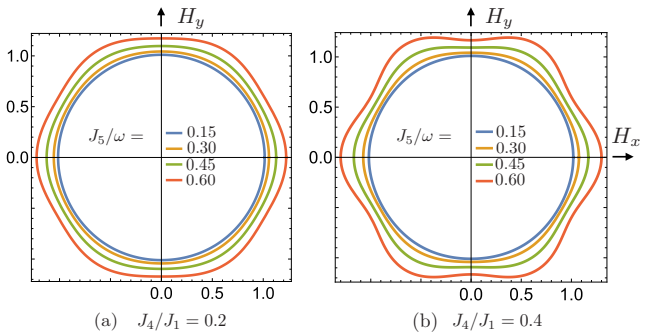

FIG. 1. Upper critical field (H_{c2}) anisotropy of two-component pairing in trigonal crystals with D_{3d} point group symmetry, originating from the trigonal GL anisotropy term (4). (a) Polar plot of the angular dependence of H_{c2} with sixfold symmetry given by Eq. (10) (normalized by $\widetilde{H}_{c2}$) for $J_4/J_1 = 0.2$. Different curves correspond to $J_5/\omega = J_5/\sqrt{J_1 J_3} = (0.15,0.30,0.45,0.60)$ (inward to outward). (b) Same as (a) but for $J_4/J_1 = 0.4$.

the form

$$F(x) = \frac{(1-x^2)^{\frac{5}{2}}}{x^2} \sum_{m\geqslant 0}^{\infty} \frac{(2m)!}{(m!)^2 4^m} \frac{x^{2m}\left(2m - \frac{x^2}{1-x^2}\right)^2}{2m + x(2m+1)}$$
$$= \frac{1-x}{x}\left[\sqrt{\frac{1+x}{1-x}}\, {}_2F_1\left(\tfrac{1}{2}, \tfrac{a}{2}; 1 + \tfrac{a}{2}; x^2\right) - 1\right], \quad (11)$$

where $a = x/(1+x)$ and ${}_2F_1[\alpha,\beta;\delta;\gamma]$ is a hypergeometric function. The function $F(x)$ has the property $F(0) = 1$, which implies that for $J_4 = 0$ (corresponding to $\omega_-/\omega_+ = 0$) no angular dependence of H_{c2} exists. The latter is a consequence of an emergent rotational symmetry of $f_{D,\text{trig}}$ in Eq. (4): It is invariant under in-plane rotations of the order parameters and coordinates according to $q_+ \to q_+ e^{2i\varphi}$, $\eta_+ \to \eta_+ e^{-i\varphi}$. (Note that this is not a physical symmetry.)

In general, however, considering all regimes of gradient coefficients that satisfy the stability constraints of the free energy, H_{c2} exhibits a sixfold anisotropy in the basal plane of the crystal. For instance, the sixfold H_{c2} anisotropy can be obtained starting from a solution of the GL equations derived from Eqs. (3) and (4) for $J_5 \neq 0$ and $J_4 = 0$, and treating J_4 as a small perturbation. This case was considered in Ref. [31] and is described in Sec. II B 2 of the SM [47].

Figure 1 shows the angular dependence of the upper critical field for small to moderate $J_5/\omega = J_5/\sqrt{J_1 J_3}$ and J_4/J_1 as obtained from Eq. (10). Note that in general, for materials with weak to moderate (crystal) anisotropy effects, one expects $J_1 \sim J_3$. To make the interplay between J_4 and J_5 explicit, we expand Eq. (10) for small J_4/J_1 and find

$$\frac{H_{c2}(\theta)}{H_{c2}(\frac{\pi}{4})} = 1 + h\cos 6\theta, \quad (12)$$

where $h = 3|J_4|J_5^2/16J_1^2 J_3$. This expression serves to highlight an important feature of the angular dependence of H_{c2}: $H_{c2}(\theta = \pi/2)/H_{c2}(\theta = 0) < 1$, which is independent of system specific parameters. Here $\theta = 0$ is defined by an axis orthogonal to a mirror plane.

Within weak coupling, the GL coefficients J_i can be obtained in terms of Fermi surface and gap function properties using a microscopic mean-field Hamiltonian with pairing potential $\hat{\Delta}(\vec{k})$ given by Eq. (1). The gradient coefficients J_1, J_3, J_4, and J_5 are proportional to $N(\varepsilon_F)v_F^2/T_c^2 \sim N(\varepsilon_F)\xi_0^2$, where ε_F, v_F, and ξ_0 are the Fermi energy, Fermi velocity, and correlation length, respectively, and $N(\varepsilon_F)$ is the density of states. (The calculations are presented in detail in Sec. III of the SM [47].) We find that their relative strength depends on the crystal anisotropy of the Fermi surface and of the gap functions $\hat{\Delta}_{1,2}(\vec{k})$. In particular, J_5 is nonzero only when trigonal Fermi surface anisotropy is present, or when the gap function is composed of trigonal crystal spherical harmonics of the E_u pairing channel (see Sec. III A of the SM [47]), and is generally expected to be weak.

The general sixfold basal plane anisotropy of H_{c2} is a direct consequence of trigonal symmetry and a discriminating characteristic of two-component pairing symmetry. Indeed, single-component superconductivity corresponding to one-dimensional pairing channels of point group D_{3d} cannot exhibit sixfold H_{c2} anisotropy: The in-plane gradient term is given by $\tilde{J}_1|D_i\psi|^2$ and has emergent U(1) rotational symmetry. As a result, the sixfold anisotropy provides a clear experimental evidence for two-component pairing.

IV. NEMATIC SUPERCONDUCTIVITY AND UPPER CRITICAL FIELD

Within our GL theory, the rotational symmetry breaking superconducting state reported in Refs. [22,23] corresponds to a *real* order parameter, i.e., $\eta = \eta_0(\cos\phi, \sin\phi)^T$. Up to fourth order [see Eq. (2)], the angle ϕ represents a continuous degeneracy. This degeneracy is lifted at sixth order by a crystal anisotropy term and leads to a discrete set of degenerate ground states [24,38]. In materials, such as $Cu_xBi_2Se_3$, the remaining degeneracy may be further lifted by a symmetry-breaking pinning field, selecting a unique ground state. The origin of such pinning can be strain-induced distortions of the crystal [44], but in principle, any order with the same symmetry, electronic or structural, can pin the order parameter. In case of two-component superconductors, the symmetry-breaking (SB) pinning field couples *linearly* to order parameter η in the following way

$$f_{\text{SB}} = g[(u_{xx} - u_{yy})(|\eta_1|^2 - |\eta_2|^2) + 2u_{xy}(\eta_1^*\eta_2 + \eta_2^*\eta_1)], \quad (13)$$

with coupling constant g. The order parameter bilinears $(|\eta_1|^2 - |\eta_2|^2, \eta_1^*\eta_2 + \eta_2^*\eta_1)$ constitute a two-component subsidiary nematic order parameter [24] with the same symmetry as the symmetry-breaking field $(u_{xx} - u_{yy}, 2u_{xy})$. For comparison, uniaxial strain in single-component superconductors couples to the gradient of the order parameter ψ, taking the form $\tilde{J}_{1,x}|D_x\psi|^2 + \tilde{J}_{2,y}|D_y\psi|^2$ different from Eq. (13). It is worth noting that the coupling considered here differs from the candidate theories proposed for the hexagonal superconductor UPt_3, in which case magnetic order couples quadratically, instead of linearly, to order parameter bilinears [27,30,39,40,45,46].

From a microscopic perspective, the origin of the order parameter pinning in Eq. (13) can be understood as a (strain-induced) Fermi surface distortion, leading to different Fermi velocities $v_{F,x} \neq v_{F,y}$. A uniaxial distortion of this form couples to $|\eta_1|^2 - |\eta_2|^2$ and has the effect of selecting either $\eta = (1,0)$ or $\eta = (0,1)$ by raising T_c, resulting in a split transition. A quantitative calculation of the coupling constant g, relating the order parameter bilinear to such Fermi surface distortion can be obtained within weak coupling (see Ref. [47]). This effect of a Fermi surface distortion should be compared to uniaxial gradient anisotropies such as $\sim|D_x\eta_a|^2 - |D_y\eta_a|^2$ and $\sim|D_i\eta_1|^2 - |D_i\eta_2|^2$, with the effect of the former being enhanced by a factor of $\ln(\omega_D/T_c)(\xi/\xi_0)^2$ [47], where ξ is the coherence length, $\ln\omega_D/T_c \sim 1/VN(\varepsilon_F)$, ω_D is a cutoff frequency, and V is an effective interaction energy scale associated with the pairing. In addition, the effect of a uniaxial Fermi surface distortion $\sim v_{F,x}/v_{F,y}$ on the shift of T_c is enhanced by $\ln\omega_D/T_c$.

To address the effect of the SB field on H_{c2} in case of the trigonal nematic superconductors, we solve the linearized GL equations for small $J_{4,5}$ gradient coefficients in the presence of a uniaxial symmetry breaking term defined as $\delta(|\eta_1|^2 - |\eta_2|^2)$, taking δ as a measure of the uniaxial anisotropy. Here we focus the discussion on the most salient features, for which we take $J_5 = 0$, and relegate a more detailed account to the SM [47]. A similar problem of upper critical field anisotropy was studied for split transitions in UPt_3 [32,33].

Setting $J_5 = 0$ in Eq. (7) and adding the contribution from the symmetry breaking field, the GL equations take the form

$$-A\eta_a = \left(J_1 D_\perp^2 + J_3 D_z^2\right)\eta_a + \delta\tau^z_{ab}\eta_b - J_4 D_\perp^2\left(\cos 2\theta\,\tau^z_{ab} + \sin 2\theta\,\tau^x_{ab}\right)\eta_b. \quad (14)$$

The upper critical field is obtained by using the magnetic algebra of D_z and $D_\perp$, and projecting into the lowest Landau level. The upper critical field is then determined from the following implicit equation (see Sec. II D of the SM [47])

$$\frac{-A}{\omega} = \frac{1}{l_b^2} - \sqrt{\frac{J_4^2 J_3^2}{4\omega^4 l_b^4} + \frac{\delta^2}{\omega^2} - \frac{J_4 J_3 \delta}{\omega^3 l_b^2}\cos 2\theta}, \quad (15)$$

(recall $\omega = \sqrt{J_1 J_3}$) where the magnetic length l_b is defined as $2eH = 1/l_b^2$. For $\delta = 0$ we recover the result for $J_5 = 0$ in Eq. (10), to first order in J_4/J_1 (i.e., ω_1 expanded to first order in J_4/J_1). For $J_4 = 0$ we simply find $H_{c2} = H_{c2,0}$ [see Eq. (12)], but with critical temperature $T_c^* = T_c + \Delta T_c$ with $\Delta T_c \sim |\delta|$. This follows from comparing δ to $A \sim (T - T_c)$, i.e., δ shifts the transition temperature and can be taken as a measure of T. We define a dimensionless temperature t by $T = T_c^* - t\Delta T_c$.

For general J_4/J_1 and nonzero δ we solve Eq. (15) for H_{c2} and show the representative results for $J_4/J_1 = 0.1$ and $J_4/J_1 = 0.6$ in Figs. 2(a) and 2(b). Two key characteristics of H_{c2} in the presence of a pinning field are evident in Figs. 2(a) and 2(b). First, the angular dependence of H_{c2} exhibits a distinct two-fold anisotropy, with a typical "peanut"-shape close to T_c^*. This twofold anisotropy becomes more pronounced with increasing J_4/J_1, as shown Fig. 2(b). Expanding the square root in Eq. (15) under the assumption of very small fields, i.e., $l_b^2 \gg J_4 J_3/2\omega\delta$, one finds $H_{c2} \propto (1 - J_4\mathrm{sgn}(\delta)\cos 2\theta/2J_1)$

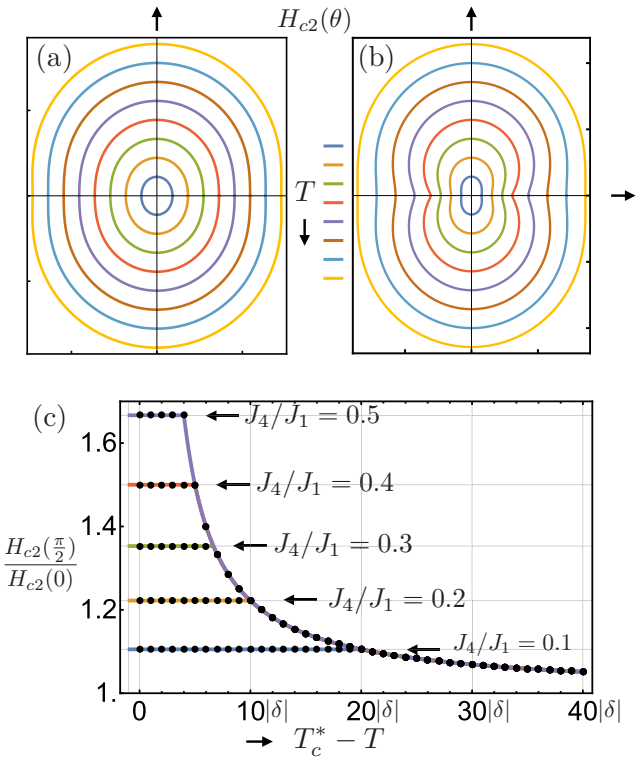

FIG. 2. (a) Polar plot of the angular dependence of H_{c2} in the presence of a symmetry-breaking field δ for $J_4/J_1 = 0.1$, calculated using Eq. (15) (in arbitrary units of H). Different curves represent different temperatures: $T = T_c^* - t\Delta T_c$ (recall that $\Delta T_c \sim |\delta|$), where $t = 1, \ldots, 8$ and the outermost curve corresponds to $t = 8$. (b) Same as in (a) but for relatively large $J_4/J_1 = 0.6$. Figure (b) clearly shows the twofold "peanut"-shape anisotropy expected for two-component superconductors in the presence of a symmetry breaking field. (c) Plot of the H_{c2}-anisotropy coefficient $H_{c2}(\frac{\pi}{2})/H_{c2}(0)$ as function of effective temperature t for various values of J_4/J_1. The horizontal grid lines correspond to the values $(1 + J_4/2J_1)/(1 - J_4/2J_1)$.

(see Sec. II D of the SM [47]). This "peanut' shape of the H_{c2} profile should be contrasted with the H_{c2} profile of single-component superconductor where uniaxial gradient anisotropy leads to a weak *elliptical* angular dependence of H_{c2}, an effect which is parametrically smaller than the twofold anisotropy in the two-component case. Consequently, the twofold anisotropy of H_{c2} shown in Fig. 2, in particular the "peanut" shape, is a discriminating property of two-component pairing.

Second, the angular dependence of H_{c2} is a function of temperature and has a different shape in the vicinity of T_c^* (i.e., small fields) as compared to far below T_c (and high fields). This is in sharp contrast to the usual case, for instance Eq. (10), where only the overall magnitude of H_{c2} is temperature dependent. The unusual temperature dependence of H_{c2} can be more precisely captured by considering the upper critical field anisotropy ratio $H_{c2}(\frac{\pi}{2})/H_{c2}(0)$ as a function of temperature. In the vicinity of T_c^*, the anisotropy ratio should exhibit temperature independent behavior given by $\sim(1 + J_4\mathrm{sgn}(\delta)/2J_1)/(1 - J_4\mathrm{sgn}(\delta)/2J_1)$ (see Sec. II D of the SM [47]). This is shown in Fig. 2(c), where the H_{c2}-anisotropy ratio is plotted for various values of J_4/J_1. In contrast, using

Eq. (15) we find that the H_{c2}-anisotropy ratio approaches unity for large temperature t according to $\sim 2/(t-1)$, which is independent of GL parameters. Within the model of Eq. (15), the temperature at which the transition between two behaviors occurs is given by $t = 2J_1/|J_4|$. This "kink" feature was also found and discussed in the context of a hexagonal applicable to UPt_3 [32,33,48]. The distinctive temperature dependence of H_{c2} anisotropy is uniquely associated with two-component pairing since single-component pairing with uniaxial gradient anisotropy leads to temperature independent H_{c2} anisotropy.

V. DISCUSSION AND CONCLUSION

To summarize, in this paper we have addressed the magnetic properties of two-component superconductors in trigonal crystals with point group D_{3d} symmetry. Starting from a general GL theory of trigonal two-component superconductors, we find that the upper critical field exhibits a *sixfold* anisotropy in the basal plane, which is a discriminating property of two-component pairing. The sixfold anisotropy is a rare manifestation of discrete crystal symmetry, since effects of crystal anisotropy are typically obscured in GL theory by an emergent U(1) rotational symmetry. In addition, in this paper we show that when a symmetry breaking field originating from, e.g., structural distortions selects a *real* order parameter, H_{c2} exhibits a twofold anisotropy with characteristic angular and temperature dependence.

The recent NMR and specific heat measurements on $Cu_xBi_2Se_3$, which reported spontaneously broken rotational symmetry, indicate that this material belongs to the class of superconductors with two-component pairing symmetry. Prominent other examples of materials with trigonal symmetry, which have attracted increasing attention recently, are the doped Bi_2Se_3 superconductors $Sr_xBi_2Se_3$, $Nb_xBi_2Se_3$, and $Tl_xBi_2Te_3$. Our theory of in-plane anisotropy of upper critical field stands to contribute to uncovering the pairing symmetry of these superconductors, which remains to be determined.

ACKNOWLEDGMENTS

We thank Anne de Visser, Shingo Yonezawa, and Yoshi Maeno for discussions. This work is supported by the David and Lucile Packard Foundation (L.F.), the DOE Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DESC0010526 (V.K.), and the Netherlands Organization for Scientific Research (NWO) through a Rubicon grant (J.V.).

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