Criterion for Vestigial Order above a Nematic Superconductor

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A nematic superconductor can in principle support a vestigial order phase above its superconducting transition temperature, with rotational symmetry spontaneously broken while remain non-superconducting. We examine the condition for this vestigial nematic order to occur, within a Ginzburg-Landau theory with order parameter fluctuations included. Contrary to prior theoretical results, we found that this vestigial order actually requires very stringent conditions to be met: the material must be sufficiently deep in the nematic regime (i.e. far away from the boundary separating the nematic and chiral superconducting phases) to possibly exhibit a vestigial nematic order.

I. INTRODUCTION

Superconductivity in doped topological insulator Bi$_2$Se$_3$ has captured much recent attention. While the crystal is supposed to have D$_{3d}$ symmetry, it has been found experimentally that the NMR Knight shifts \[^1\] and the upper critical fields \[^2\] have two-fold anisotropy in the basal plane. These are explained by the proposal that superconductivity in this system is nematic \[^3\]. More precisely, it has been proposed that the superconducting order parameter belongs to a two-dimensional representation, and the energetics is such that, below the superconducting transition, the order parameter picks a state with spontaneously broken rotational symmetry (other than the other possibility where time reversal symmetry is broken, \textit{c.f.} the case for UPt$_3$ \[^4, 5\]). Two-fold symmetry breakings have been observed also in many other experiments, as reviewed in \[^6\].

If the order parameter belongs to a two-dimensional representation, one expects an internal degree of freedom, in this case, rotation of the order parameter, to reveal itself under suitable circumstances. However, so far no experiments have convincingly shown this degree of freedom. One may expect external stress can re-orient the order parameter \[^7\], but an experiment at Argonne \[^8\] turns out to be negative. In a related experiment on multidomain sample at Kyoto \[^9\], only changes of the sample as a function of temperature or field were monitored. A rapid and directional dependent change as a function of temperature above the superconducting transition was observed and interpreted as a step indicating a first order transition into a vestigial nematic order state. It is remarkable that the relative change in length is only of order $10^{-7}$, even smaller than the distortion from perfect D$_{3d}$ found at higher temperatures from another group \[^10\]. Vestigial orders have been recently discussed in many other systems \[^11, 12\].

In a Ginzburg-Landau formulation, superconducting order parameter belonging to a two-dimensional representation in a D$_{3d}$ system has two “interacting” constants, or coefficients entering the quartic terms of the free energy. (e.g. $\beta_{1,2}$ in our notations \[^13\] below). These parameters dictate whether the mean-field superconducting ground state of the system would have nematic order (in our case $-\beta_1 < \beta_2 < 0$) or broken time-reversal

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\[^3\] A nematic superconducting order parameter breaks both gauge and rotational symmetry. In principle these two broken symmetries do not necessarily occur at the same temperature. A few years ago, \[^17\] predicted that “vestigial nematic order” can exist in this system: as the temperature is lowered, the symmetry preserving normal state first makes a transition into a state with broken rotational symmetry, and only later gauge symmetry is broken, forming the nematic superconducting state. This possibility is unique to a multi-component order parameter: a superconductor with an order parameter belonging to a one-dimensional representation, even if it is not s-wave, cannot exhibit this vestigial order. Observation of this “vestigial nematic state” would be a “smoking gun” of this nature of the order parameter. Not long after this proposal, an experiment \[^18\] indeed claimed that this vestigial order has been observed. In particular, length change of the sample as a function of temperature or field was monitored. A rapid and directional dependent change as a function of temperature above the superconducting transition was observed and interpreted as a step indicating a first order transition into a vestigial nematic order state. It is remarkable that the relative change in length is only of order $10^{-7}$, even smaller than the distortion from perfect D$_{3d}$ found at higher temperatures from another group \[^19\]. Vestigial orders have been recently discussed in many other systems \[^20, 21\].

In a Ginzburg-Landau formulation, superconducting order parameter belonging to a two-dimensional representation in a D$_{3d}$ system has two “interacting” constants, or coefficients entering the quartic terms of the free energy. (e.g. $\beta_{1,2}$ in our notations \[^13\] below). These parameters dictate whether the mean-field superconducting ground state of the system would have nematic order (in our case $-\beta_1 < \beta_2 < 0$) or broken time-reversal
symmetry ($\beta_2 > 0$). Ref. [17], analyzing the problem using a Hubbard-Stratanovich transformation, concluded that all regions with $-\beta_1 < \beta_2 < 0$ with a nematic superconducting ground state can potentially exhibit vestigial nematic order above the superconducting transition temperature (though in some circumstances they found “joint first order superconducting transition”). In this paper, we offer several different arguments showing that a much stronger necessary condition is needed for vestigial nematic order, namely $-\beta_1 < \beta_2 < -\beta_1/2$. (See Fig. 1). Hence only systems with parameters “deep” in the mean-field nematic region can exhibit vestigial order. For $-\beta_1/2 < \beta_2 < 0$ direct transition from the normal state through a second order transition into a superconducting nematic state is expected. Hence the experimental interpretation of [18] of vestigial nematic order would necessarily require a microscopic theory with parameters in that “deep nematic region”, placing much stronger constraint on the theory themselves than the current literature realizes. More discussions on this will be given near the end of this paper.

For $\beta_2 > 0$, while $\beta_2 < 0$, sequences in mean field, stability requires $\beta_1 > 0$, while $\beta_2 > -\beta_1$. For $T < T_0$, the superconducting nematic state is the mean-field ground state if $\beta_2 < 0$, whereas if $\beta_2 > 0$ a superconducting state with broken time reversal symmetry would be favored. Stability of the uniform state also restricts the coefficients $K_{1,2,3}$ and $K'$: we shall return to those conditions below.

If we follow [17] and introduce the column vector

$$\eta = \left( \begin{array}{c} \eta_x \\ \eta_y \end{array} \right),$$

eq (3) can be written as

$$H_{int} = \frac{\beta_1}{2} (\eta_x^* \eta_x) + \frac{\beta_2}{2} (\eta_y^* \eta_y)$$

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The rest of the paper are as follows. In Sec II we analyze the vestigial order, using a variational method. Besides obtaining the condition for vestigial order mentioned just above, we also provide more details on this vestigial transition and the superconducting transitions. Sec III provides a conclusion. In Appendix A we evaluate the nematic susceptibility which gives the same criterion for vestigial order as in Sec III. Appendix B contains some mathematical details, as well as further discussions on parameteric dependences which we have left out in the text.

II. THEORY FOR VESTIGIAL ORDER

The effective Hamiltonian density

$$\mathcal{H} = \mathcal{H}_K + \mathcal{H}_{int}$$

consists of two parts. The “kinetic” part

$$\mathcal{H}_K = \alpha (\eta_x^* \eta_x) + K_1 (\partial_i \eta_x)^* (\partial_i \eta_y) + K_2 (\partial_i \eta_y)^* (\partial_i \eta_y) + K_3 (\partial_i \eta_x)^* (\partial_i \eta_y) + K_{zz} (\partial_z \eta_x)^* (\partial_z \eta_y)$$

$$+ \frac{K'}{2} [(\partial_z \eta_x^*)(\partial_x \eta_x - \partial_y \eta_y) + (\partial_z \eta_y^*)(\partial_x \eta_y + \partial_y \eta_x) + h.c.]$$

(2)

together with the “interacting” part

$$\mathcal{H}_{int} = \frac{\beta_1}{2} (\eta_x^* \eta_x) + \frac{\beta_2}{2} (\eta_y^* \eta_y)$$

(3)
the second form is the same as that in [17]. Within mean-field theory, the ground state for \( \beta_2 < 0 \) correspond to the column vector \( \eta \) being finite and real up to an overall phase factor. In this case, both the rotational symmetry and gauge symmetry are simultaneously broken. The vestigial nematic phase however correspond to the case where the expectation value of this superconducting order parameter vanishes, yet with the expectation values of \( \langle \tau^x \rangle = |\eta_x|^2 - |\eta_y|^2 \) and \( \langle \tau^y \rangle = \eta_x^* \eta_y + \eta_y^* \eta_x \) not both zero. The finiteness of these expectation values indicate that the rotational symmetry of the system has been broken. [3, 17]

In this notation, \( H_K \) after Fourier transform reads

\[
H_K = \eta \left( \alpha + \epsilon_0(\vec{K}) + \vec{\epsilon}(\vec{K}) \cdot \tau \right) \eta \quad (7)
\]

\( \epsilon_0(\vec{K}) = K(k_x^2 + k_y^2) + K_{zz}k_z^2 \) with \( K \equiv K_1 + K_{2z}, \) only has \( x \) and \( z \) components, with \( \epsilon'_x = K_{23}k_x k_y + K'k_z k_y, \) \( \epsilon'_y = K_{23}k_y k_y + K'k_z k_y, \) \( K_{23} = K_2 - K_3. \) We shall assume that, within mean-field theory, uniform states are stable even at \( T_0, \) hence for all \( \vec{K} \neq 0, \) \( c_0 > 0, \) and \( c_0^2 - c^2 > 0. \)

As we shall see, it is convenient to introduce

\[
\Phi = \left( \begin{array}{c} \Phi_\uparrow \\ \Phi_\downarrow \end{array} \right) = \frac{1}{\sqrt{2}} \left( \begin{array}{c} \eta_x + i\eta_y \\ \eta_x - i\eta_y \end{array} \right) \quad (8)
\]

The fields \( \Phi_{\uparrow, \downarrow} \) are, up to a factor of \( \sqrt{2}, \) same as the \( \eta \) used in our earlier paper [13]. The transformation from \( \eta \) to \( \Phi \) is similar to a different choice of quantization axis for a spin 1/2 wavefunction, and we shall indeed see that it is advantageous to view \( \Phi \) as just forming such an object. [25] In this new basis, the kinetic part of the energy becomes

\[
H_K = \Phi \left( \alpha + \epsilon_0(\vec{K}) + \vec{\epsilon}(\vec{K}) \cdot \vec{\sigma} \right) \Phi \quad (9)
\]

\( \vec{\sigma} \) are the Pauli matrices in space of [35]. \( \epsilon_0(\vec{K}) \) is the same as before, \( \vec{\epsilon} \) now only has \( x \) and \( y \) components, with \( \epsilon_x = K_{23}k_x k_y + K'k_z k_y, \) \( \epsilon_y = -K_{23}k_y k_y - K'k_z k_y. \) In this same basis, the interaction part of the Hamiltonian now reads

\[
H_{int} = \frac{g_1}{2}(|\Phi_{\uparrow}|^4 + |\Phi_{\downarrow}|^4) + g_2(|\Phi_{\uparrow}|^2|\Phi_{\downarrow}|^2) \quad (10)
\]

where \( g_1 = \beta_1, \) \( g_2 = \beta_1 + 2\beta_2. \) Now \( g_1 > 0, \) \( g_2 > -g_1 \) for stability, and the mean-field superconducting nematic phase is the ground state if \( g_2 < g_1. \) (See Fig 1.) A general mean-field order parameter in this state is \( \Phi \) with \( |\Phi_\uparrow| = |\Phi_\downarrow|. \) For the vestigial nematic phase, the expectation value \( \langle \Phi \rangle \) of the superconducting order parameter vanishes while \( \langle \Phi^* \sigma_{x,y} \Phi \rangle \) are not simultaneously zero. Alternatively, the expectation value \( \langle \Phi^* \Phi \rangle \) is finite. If we write \( \Phi_{\uparrow, \downarrow} = |\Phi_{\uparrow, \downarrow}| e^{i\chi_{\uparrow, \downarrow}} \) and \( \chi_{\uparrow, \downarrow} = \chi + (-)^{\nu_{\uparrow, \downarrow}} \) with \( \chi \) an overall phase and \( \chi \) a relative phase, this vestigial state can be understood as one where \( \chi \) is disordered whereas the relative phase angle \( \chi \) is ordered.

This state thus bears a strong similarity with the “metallic superfluid” state studied in, e.g. [26] or the “counterflow superfluid” in [27] with here \( \Phi_\uparrow \) and \( \Phi_\downarrow \) playing the role of the two \( U(1) \) components there. Now however \( \chi \) contains information about the spatial direction in the \( x - y \) plane along which the rotational symmetry is broken (and the mechanisms considered in [26, 27] are also different).

The advantage of this new basis is now obvious. As said, one can just view the system as an effective spin-1/2 system. The gradient coupling (9) consists of a part \( \vec{\epsilon} \) which can be regarded as a kind of spin-orbit coupling. The interaction (10) in general has an XXZ symmetry. From eq (10), it is highly suggestive that the crucial parameter which determines the “locking” the relative phase between the \( \uparrow, \downarrow \) components is \( g_2, \) as we shall indeed verify below. This result is also supported by an examination of the “nematic susceptibility” in App A.

We remind the reader that \( g_2 = 0 (\beta_2 = -\beta_1/2) \) corresponds to a point “in the middle” within the mean-field nematic region \( -g_1 < g_2 < g_1 \) \( (\beta_1 < \beta_2 < 0). \) We shall see that it is a dividing point between where the vestigial nematic order can exist or not. (See Fig 1.) In contrast, [17], employing a Hubbard-Stratanovich transformation, proposed that all regions with \( \beta_2 < 0 \) can potentially exhibit vestigial nematic order. However, the decomposition of the quartic interaction terms is not unique (c.f. [5, 6] and (10)), so it is conceivable that an incorrect answer can be obtained. We also note that, in the absence of \( \vec{\epsilon} \) and \( g_2, \) then the up and down components are completely decoupled, and the system has an enhanced \( U(1) \times U(1) \) symmetry, where the two \( U(1)’s \) correspond to gauge transformations of the up and down components respectively. In this limit vestigial nematic order would be trivially absent. (For completeness, though not directly related to the problem we currently have, we mention that \( g_2 = g_1 \) would correspond to a hidden \( SU(2) \) symmetry; not surprising since at that point the nematic and broken time reversal symmetry states are degenerate).

To investigate the vestigial nematic order, we employ a variational approach (see, e.g., [28]), which has also been adopted before by, e.g., [20] to study the vestigial order in the broken time-reversal symmetry case [20]. In this method, in contrast to the Hubbard-Stratanovich transformation mentioned above, one does not have to rely on a particular choice of writing the quartic interaction terms and an identification of which way one is making the decomposition. There exist, however, important differences between our treatment and [20], on which we shall comment when we proceed. The free energy \( F \) of a system obeys the inequality

\[
F \leq F_0 + \langle H - H_0 \rangle_0 \quad (11)
\]

where \( H_0 \) is an ansatz Hamiltonian, \( F_0 \) the corresponding free energy, and the angular brackets denote thermodynamic average performed with respect to the ansatz \( H_0, \) i.e., with the weighting factor according to \( e^{-\beta H_0}, \) where
$T$ is the temperature. In the notation $\Phi$, the vestigial order corresponds to a broken in-plane spin symmetry, hence we adopt the ansatz

$$\mathcal{H}_0 = \mathcal{H}_K - \Phi^\dagger(\vec{h} \cdot \vec{\sigma})\Phi$$

(12)

where the in-plane vector $\vec{h}$ ($h_z = 0$) contains our variational parameters $(h_{x,y})$.

The calculation can be done by noting that

$$\langle \Phi^*_{\vec{k},s} \Phi_{\vec{k}',s'} \rangle_0 \equiv TG_{ss'}(\vec{k})$$

(13)

with the “Green’s function” $G$ whose inverse is given by

$$G(\vec{k}) = \alpha + \epsilon_0 + (\vec{\epsilon} - \vec{h}) \cdot \vec{\sigma}$$

(14)

Hence

$$G(\vec{k}) = \frac{\alpha + \epsilon_0 - (\vec{\epsilon} - \vec{h}) \cdot \vec{\sigma}}{\mathcal{D}} \equiv G_0 + \vec{G} \cdot \vec{\sigma}$$

(15)

with

$$\mathcal{D}(\vec{k}) \equiv (\alpha + \epsilon_0)^2 - (\vec{\epsilon} - \vec{h})^2$$

(16)

$F_0$ is simply given by

$$F_0(\vec{h}) = T \sum \ln \mathcal{D}(\vec{k}) \ .$$

(17)

Let us write $\mathcal{H}_1 \equiv g_1(|\Phi|^4 + |\Phi|^4)$ and $\mathcal{H}_2 \equiv g_2(|\Phi|^2|\Phi|^2)$. Now $\langle H - H_0 \rangle_0 = \langle H_1 \rangle_0 + \langle H_2 \rangle_0$ plus $\langle \Phi^\dagger\vec{h} \cdot \vec{\sigma}\Phi \rangle_0$, with

$$\langle H_1 \rangle_0 = g_1 \sum_{\vec{k},\vec{k}'} \langle \Phi^*_{\vec{k},s} \Phi_{\vec{k}',s} \rangle_0 \langle \Phi^*_{\vec{k}',s'} \Phi_{\vec{k},s'} \rangle_0$$

$$= 2g_1 T^2 \sum \mathcal{D}(\vec{k}) \sum \mathcal{D}(\vec{k}')$$

(18)

$$\langle H_2 \rangle_0 = \langle H_{21} \rangle_0 + \langle H_{22} \rangle_0$$

(19)

consists of a “longitudinal” contribution

$$\langle H_{21} \rangle_0 = g_2 \sum_{\vec{k},\vec{k}'} \langle \Phi^*_{\vec{k},s} \Phi_{\vec{k}',s} \rangle_0 \langle \Phi^*_{\vec{k}',s'} \Phi_{\vec{k},s'} \rangle_0$$

$$= 2g_2 T^2 \sum \mathcal{D}(\vec{k}) \sum \mathcal{D}(\vec{k}')$$

(20)

and a “transverse” piece

$$\langle H_{22} \rangle_0 = g_2 \sum_{\vec{k},\vec{k}'} \langle \Phi^*_{\vec{k},s} \Phi_{\vec{k}',s} \rangle_0 \langle \Phi^*_{\vec{k}',s'} \Phi_{\vec{k},s'} \rangle_0$$

$$= 2g_2 T^2 \sum \mathcal{D}(\vec{k}) \sum \mathcal{D}(\vec{k}')$$

(21)

and

$$\langle \Phi^\dagger(\vec{h} \cdot \vec{\sigma})\Phi \rangle_0 = 2T \vec{h} \cdot \sum \vec{G}(\vec{k}) \ .$$

(22)

Note that our $H_{1,2}$ have been treated similarly.

In order to see the roles of the different terms and for a closer comparison with [17], we shall consider the various contributions to $F$ separately. Readers who are not interested in these details can simply note the definitions [24], [25], [26], [27] and [30] below and directly skip to eq (37) for the final expression for the free energy. We first consider only the contributions from $F_0$ (eq (17)) $\langle H_{21} \rangle$ (eq (21)), and $\langle \Phi^\dagger(\vec{h} \cdot \vec{\sigma})\Phi \rangle$ (eq (22)). We expand them in $\vec{h}$. For $F_0$, we get

$$F_0(\vec{h}) = F_0(0) + a(h_x^2 + h_y^2) + \frac{2b}{3}(h_x^3 - 3h_xh_y^2) + \frac{c}{2}(h_x^2 + h_y^2)^2$$

(23)

where we have defined

$$\mathcal{D}(\vec{k}) \equiv (\alpha + \epsilon_0)^2 - (\vec{\epsilon} - \vec{h})^2$$

(24)

$$a = -T \sum \left[ \frac{1}{\mathcal{D}(\vec{k})} + \frac{\epsilon^2}{\mathcal{D}(\vec{k})} \right]$$

(25)

$$b = \frac{8}{3} T \sum \frac{\epsilon^3}{\mathcal{D}(\vec{k})}$$

(26)

$$c = -T \sum \left[ \frac{1}{\mathcal{D}(\vec{k})^2} + \frac{\epsilon^2}{\mathcal{D}(\vec{k})^2} + \frac{\epsilon^4}{\mathcal{D}(\vec{k})^4} \right]$$

(27)

In obtaining eq (23), we have made use of the $D_{3d}$ symmetry of the crystal to relate some of the sums (See App B). We also remark that $b$ is non-zero only when $K'$ is finite (see also App B). We note that eq (23) obeys $D_{3d}$ symmetry, in particular, $(h_x^3 - 3h_xh_y^2)$ is an allowed cubic invariant, as it remains the same under rotation by $2\pi/3$ about the z axis and rotation by $\pi$ about x.

In eqs (21) and (22), we need also the sums $T \sum \mathcal{D}(\vec{k})$. On noting that $d\mathcal{D}/dh_x = 2(\epsilon_x - h_x)$ and recalling eq (15), we see that they can be obtained simply by differentiating $T \sum \ln \mathcal{D}(\vec{k})$ hence eq (23) with respect to $h_{x,y}$ and then multiplying by $-1/2$. We get eventually
\[ \langle H_{2a}\rangle_0 = g_2 \left[ a^2(h_x^2 + h_y^2) + 2ab(h_x^3 - 3h_xh_y^2) + (2ac + b^2)(h_x^2 + h_y^2)^2 \right] \] (28)

and

\[ \langle \Phi^4(\tilde{h} \cdot \vec{\sigma})\Phi \rangle_0 = -2a(h_x^2 + h_y^2) - 2b(h_x^3 - 3h_xh_y^2) - 2c(h_x^2 + h_y^2)^2. \] (29)

These three contributions \( F_0, \langle H_{2a}\rangle, \) and \( \langle \Phi^4(\tilde{h} \cdot \vec{\sigma})\Phi \rangle_0 \) together give an interim free energy, which we shall call \( F_{\text{interim},}\)

\[ F_{\text{interim}}(\tilde{h}) = F_{\text{interim}}(0) + [a(g_2a - 1)](h_x^2 + h_y^2) + [b(2g_2a - \frac{4}{3})](h_x^3 - 3h_xh_y^2) + [g_2(2ac + b^2) - \frac{3c}{2}](h_x^2 + h_y^2)^2. \] (30)

Let us analyze \( F_{\text{interim}} \) and pretend this is the full expression for \( F \) at the moment. Let us first note that, for temperatures above the mean field transition temperature \( T_0, \alpha > 0 \) and hence \( a \) is negative definite. We see that if \( g_2 > 0 \), the coefficient of the \( h^2 \) term is positive definite. \( h = 0 \) is always a local minimum and no broken symmetry state with finite \( h \) is expected for temperatures above \( T_0 \). If \( g_2 < 0 \), the situation is different. Writing it as \((-a)|g_2|(\frac{1}{g_2} + a)\), noting that since the magnitude of \( a \) increases as the temperature is lowered towards \( T_0 \) (and diverges to \(-\infty \) at \( T_0 \) where \( \alpha \to 0 \)), we see that this coefficient is positive at high temperatures, then vanishes at a “critical temperature” \( T_1 > T_0 \) where \( \tilde{a} \equiv (\frac{1}{g_2} + a) = 0 \), and changes sign below. This indicates a possible broken symmetry state above the mean-field transition temperature \( T_0 \). \( g_2 < 0 \) is required, in agreement with App A.

Let us, in the spirit of Ginzburg-Landau theory, approximate all coefficients by the value at \( T_1 \) except the coefficient of \( \tilde{h}^2 \), that is, in all terms except \( \tilde{a} \), put \( g_2a = 1 \). We get

\[ F_{\text{interim}}(\tilde{h}) \approx F_{\text{interim}}(0) + (\frac{1}{|g_2|} + a)(h_x^2 + h_y^2) + \frac{2}{3}b(h_x^3 - 3h_xh_y^2) + [g_2b^2 + \frac{c}{2}](h_x^2 + h_y^2)^2 \] (31)

At this point, it is interesting to compare this result with what we would get if we treat the \( g_2 \) interaction term by a Hubbard-Stratanovich transformation (ignoring \( \mathcal{H}_1 \) for the moment). If we write \( \mathcal{H}_2 \) as \( g_2(\Phi^4 - 1)(\Phi^4 + 1) = \frac{2g_2}{4} \sum_{\mu=x,y}(\Phi^4 + 1) \Phi^4 \) and decompose this quartic term using \( \frac{g_2}{2} \frac{\tilde{h}^2}{(-g_2)} \Phi^4 \) with \( \tilde{h} \) containing again only \( x \) and \( y \) components, we obtain an effective Hamiltonian

\[ \mathcal{H}_{\text{eff}} = \mathcal{H}\mathcal{K} - \tilde{h} \cdot (\Phi^4 \vec{\sigma} \Phi) + \frac{\tilde{h}^2}{(-g_2)} \] (32)

Now given \( \mathcal{H}_{\text{eff}} \) and \( g_2 < 0 \), the free energy is simply

\[ F_{\text{eff}} = \frac{\tilde{h}^2}{|g_2|} + T \sum_{k} \ln D(\tilde{k}) \] (33)

If we expand this expressions in \( \tilde{h} \) (noting that the last term is just the same as our \( F_0 \) in eq (17) and hence eq (28)), we obtain an expression that is identical with eq (33) except that the \( g_2 b^2 \) term (which is typically small and is absent entirely if the symmetry is slightly higher, say \( \mathcal{D}_{0h} \), see App. B) in front of \( \tilde{h}^4 \) is now absent. We can trace the reason for this similarity by noting that, if we put \( g_2a = 1 \), the sum of \( H_{2b} \) and \( \langle \Phi^4(\tilde{h} \cdot \vec{\sigma})\Phi \rangle_0 \) is just (see eqs (28) and (29)) \( \frac{\tilde{h}^2}{|g_2|} \), apart from the \( g_2 b^2 \tilde{h}^4 \) term we just mentioned (there are further differences but higher orders in \( \tilde{h} \)). Taking the derivative of eq (33) we obtain a self-consistent equation for \( \tilde{h} \), which reads

\[ \tilde{h} = g_2 T \sum_{k} \frac{\vec{e} - \tilde{h}}{D} \] (34)

This has the same form as the self-consistent equation in (17), except the important difference that the interaction coefficient appearing here is \( g_2 \), while the expression in (17) contains what is \( \beta_2 \) in our notation. This difference is an artefact of the Hubbard-Stratanovich decoupling procedure mentioned earlier: the decomposition of the quartic term depends spuriously on the way one chooses to express the term. (Also, on the right-hand-side of eq (31), instead of our \( D \) in the denominator, they have instead \( (\alpha + R + \epsilon_0)^2 - \epsilon^2 \), thus with an extra contribution \( R \). We shall comment on this difference later). We note that eq (34) implies the same condition for vestigial nemtic order as we found earlier: \( g_2 < 0 \), or \( \beta_2 < -\beta_1/2 \), rather than just \( \beta_2 < 0 \) found in (17).

However, there is a serious problem in this simplified analysis so far. While eq (30)-(34) seemingly yield the correct condition for vestigial order, we will shortly see that \( F_{\text{interim}} \) in eq (31) does not have a stable ground state. (As corollary, any theory based solely on eqs (33) and (34) must also be unstable.) We shall see that the
terms $\langle H_1 \rangle$ and $\langle H_2 \rangle$ that we have left out thus far, stabilize the theory. Note then that since $F_{\text{interim}}$ in eq (31) is not our full expression for the free energy $F$, and since $\vec{h}$ should be determined from the minimization of $F$, eq (31) is not our equation for $\vec{h}$. However, as we shall see shortly below, the $\vec{h}^2$ coefficient of $F$ is correctly given by that in eq (30) thus (31), hence it does not alter the

$$
\langle H_1 + H_{2l} \rangle = (2g_1 + g_2)T^2 \left( \sum_k (G_0)_{\vec{k} = 0} + \vec{h} \cdot \frac{\partial G_0}{\partial \vec{h}} + \ldots \right) \times \left( \sum_k (G_0)_{\vec{k} = 0} + \vec{h} \cdot \frac{\partial G_0}{\partial \vec{h}} + \ldots \right)
$$

(35)

with the $\vec{h}$ derivatives evaluated at $\vec{h} = 0$. Since $G_0 \propto 1/\vec{k}^2$ at large $\vec{k}$, we see that the sum $T \sum_k G_0 |_{\vec{k} = 0}$ is ultraviolet divergent. The $\vec{h} = 0$ contribution is however irrelevant to us since we only need to consider $F(\vec{h}) - F(\vec{h} = 0)$. There is no first order term in eq (35) as $\frac{\partial \tilde{G}_0}{\partial \vec{h}} |_{\vec{h} = 0} = -2\pi \epsilon_0 c(\vec{k})$ sums to zero due to the angular dependent $\vec{c}$. At first sight one might think there is an $\vec{h}^2$ contribution from $T^2 \sum_k G_0 |_{\vec{k} = 0} \times \left( \sum_k \frac{h_\mu h_\nu}{2} \frac{\partial^2 G_0}{\partial h_\mu \partial h_\nu} \right)$ or vice versa. However, one can easily see that these terms are just what we would get for the modifications to the $\vec{h}^2$ terms of $F_0$ if we include the one-loop self-energy terms due to $g_{1,2}$ in $G$, i.e., if we insert a self-energy $-2g_1 \langle \Phi_1(\vec{k}) \Phi_1^*(\vec{k}) \rangle |_{\vec{h} = 0} - g_2 \langle \Phi_2(\vec{k}) \Phi_2^*(\vec{k}) \rangle |_{\vec{h} = 0}$ in the $\uparrow \downarrow$ component $G^{-1}$ of eq (13) (and similarly for $\uparrow \downarrow$). Including this self-energy is equivalent to replacing $\alpha$ by $\alpha + (2g_1 + g_2)T \sum_k G_0 |_{\vec{k} = 0}$. These insertions simply renormalizes $T_0$ and $\alpha'$, that is, the mean-field transition temperature and the derivative of $\alpha$ with respect to the temperature. As in usual treatment of phase transitions (31, 32), we assume that these replacements have already been done from the outset and therefore we shall simply leave this contribution out. There are therefore no modifications to $F(\vec{h}) - F(0)$ that is second order in $\vec{h}$.

Neither there are modifications to $F(\vec{h}) - F(0)$ of third order since $\sum_k \frac{\partial \tilde{G}_0}{\partial \vec{h}} |_{\vec{h} = 0}$ vanishes as explained above. The lowest order contribution is thus fourth order in $\vec{h}$, arising from

$$
T^2 \left( \sum_k h_\mu h_\nu \frac{\partial^2 G_0}{\partial h_\mu \partial h_\nu} \right) \times \left( \sum_k \frac{h_\mu h_\nu}{2} \frac{\partial^2 G_0}{\partial h_\mu \partial h_\nu} \right). \quad \text{The factor } T^2 \left( \sum_k \frac{h_\mu h_\nu}{2} \frac{\partial^2 G_0}{\partial h_\mu \partial h_\nu} \right) \text{ is finite only for } \mu = \nu = x \text{ or } y,
$$

and we get the contribution $c' \vec{h}^4$ with (33)

$$
c' = 2(2g_1 + g_2)T^2 \left[ \sum_k \left( \frac{\alpha + \epsilon_0}{D_0} + 2 \frac{\alpha + \epsilon_0 \epsilon_2}{D_0} \right)^2 \right]^{2/3}
$$

(36)

The end result is that the free energy $F$ is given by eq (31) with an additional contribution to the fourth order term, thus

$$
F(\vec{h}) = F(0) + \tilde{a}(h_x^2 + h_y^2) + \frac{2}{3} b(h_x^3 - 3h_x h_y^2) + \frac{\tilde{c}}{2}(h_x^2 + h_y^2)^2
$$

(37)

where $\tilde{c} = c + 2g_2 b^2 + c'$. We remind the readers that $\tilde{a} \equiv \frac{1}{(2g_1 + a)}$ is positive for $T > T_1$ and negative below, with $T_1 > T_0$.

We note here all the coefficients $\tilde{a}, b, \tilde{c}$ entering eq (37) are given by sums that are ultraviolet convergent: to compute them, one needs only the information near $\vec{k} \approx 0$. This is in contrast to both (17) and (29). They both have explicitly included a term that correspond to our one-loop self-energy mentioned in the discussion below (35). This term has been removed by us by renormalization of $\alpha$. The treatment of this term in this way is also consistent with App. A.

The stability $\tilde{c} > 0$ is provided by $g_1 > 0$ if $g_1$ is sufficiently large. Let us examine this condition in more detail. The presence of $\tilde{c}$ in $D_0$ makes the analytic evaluation of the integrals difficult. Let us first simplify the problem first by pretending that the $\tilde{c}^2$ term in $D_0$ is small, and replace all $D_0$ terms in the denominators of the sums involved by $D_{00} \equiv (\alpha + \epsilon_0)^2$. We find (see App
\[c = -\frac{1}{2\pi \alpha^{5/2}} \frac{T}{K K_{zz}^{3/2}} \]  
\tag{38}

and
\[c' = 2(2g_1 + g_2) \left[ \frac{1}{2\pi \alpha^{5/2}} \frac{T}{K K_{zz}^{3/2}} \right]^2 \]  
\tag{39}

In these expressions, we have only kept the first terms in eqs. (27) and (30), ignoring the terms involving explicitly \( \tilde{c} \)'s in the same spirit as just described. Note that then, as the temperature is lowered towards the mean-field transition temperature from above, the magnitude of \( c' \) grows faster than \( c \). On the other hand, the temperature \( T_1 \) where the term \( \tilde{a} \) in \( F \) changes sign occurs at (see App B)
\[\frac{1}{|g_2|} = \frac{1}{8\pi} \frac{T_1}{\alpha(T_1)^{1/2} K K_{zz}^{3/2}}, \]  
\tag{40}

and hence
\[ (T_1 - T_0) = \frac{1}{\alpha'} (\frac{|g_2| T_1}{g_2})^2 \frac{1}{K K_{zz}^{3/2} (8\pi)^2}. \]  
\tag{41}

where on the right hand side we can also replace the explicit temperature \( T_1 \) by \( T_0 \) since the dominant temperature variation in eq. (10) arises from \( \alpha(T) \). One recognizes the right hand side has the same parametric form of the usual (Ginzburg) estimate for the width of the fluctuation region \( \tilde{g}_2 \) with \( g_2 \) playing the role of the interaction. For usual superconductors this region is expected to be small compared with the mean-field transition temperature \( T_0 \), though \( \tilde{g}_2 \) obtained a rather large value in their theory of doped \( \text{Bi}_2\text{Se}_3 \). If we replace the coefficients \( c \) and \( c' \) by their values at \( T_1 \) (in the spirit of usual Ginzburg-Landau theory), the condition \( \tilde{c} > 0 \) is equivalent to (dropping the contribution \( g_2b_0 \) in the same spirit as above) \( g_1 > |g_2| \), hence satisfied for the entire region where the mean-field theory is stable. If we include the contributions from \( \tilde{c}, \tilde{c} > 0 \) will continue to hold except perhaps for some violation near \( g_2 \approx -g_1 \).

Assuming \( \tilde{c} > 0 \), the analysis of the free energy (37) is standard. In the special case \( b = 0 \), (recall this is the case if \( K' = 0 \)) then we have a second order transition into the vestigial nematic state with \( \tilde{h} \neq 0 \) at \( T_1 \), where \( \tilde{a} \) changes sign. For the more general situation with \( b \neq 0 \), we instead obtain a first order phase transition from the normal state to the vestigial nematic state at \( \tilde{a}(T_1^*) = \frac{\tilde{h}^2}{2m} > 0 \), hence \( T_1^* > T_1 \), to the state \( \tilde{h} = h_x \hat{x} \) (or its rotated partners by \( \pm 2\pi/3 \)) with \( h_x = -\frac{\tilde{h}^2}{2m} \). \( b \) is finite only when both \( K_{23} \) and \( K' \) are finite, but is even in \( K' \) while odd in \( K_{23} \), with \( \text{sgn} b = -\text{sgn}(K_{23}) \) (see App B), hence \( \text{sgn} h_x = \text{sgn}(K_{23}) \). To be self-consistent, the above assumed that the value of \( |\tilde{h}| = |\tilde{h}(\frac{T_1}{2})| \) at \( T_1^* > T_1 \) is less than \( \alpha(T_1^* - T_1) \), so that \( D(\tilde{k}) \) at this point is still positive, else we should have a first order phase transition directly into a superconducting state with broken rotational and broken gauge symmetry. For more discussions on this condition, see App B.

Upon lowering the temperature from \( T_1^* \), \( \alpha(T) \) decreases but \( |\tilde{h}| \) increases, hence at some temperature \( T_1^* < T_c, G^{-1}(\tilde{k}) \) will have a zero eigenvalue. \( \Phi \) grows from \( 0 \) at \( T_c^* \) and increases with lowering temperature, signifying a second order transition into the superconducting state. This transition turns out to occur at \( \tilde{k} = 0 \) and at the temperature \( T_c \) where \( \alpha(T_c) = |\tilde{h}| > 0 \). To check this, consider the special case \( \tilde{h} = h_x \hat{x} \). Then \( D(\tilde{k}) = \alpha^2 - h_x^2 \), thus vanishes at \( \alpha = h_x \). For general \( \tilde{k} \), \( D(\tilde{k}) = \alpha^2 - h_x^2 + 2(\alpha_0 + h_x \epsilon_x) + (\epsilon_0^2 - \epsilon^2) \). If \( \tilde{k} \neq 0 \), the last term is positive by our assumption. At \( h_x = \alpha \), the second term is also positive due to the same criterion. Hence at \( \alpha = h_x \), \( D(\tilde{k}) > 0 \) if \( \tilde{k} \neq 0 \), hence the transition occurs at \( \tilde{k} = 0 \) as claimed.

At the transition, the superconducting state \( \Phi_{\tilde{k}=0} \) is an eigenvector of \( G^{-1}(\tilde{k} = 0) \) with a zero eigenvalue. Since at this point \( G^{-1}(\tilde{k} = 0) = \alpha - h_x \sigma^x \), we have \( h_x \sigma^x \Phi_{\tilde{k}=0} = \alpha \Phi_{\tilde{k}=0} \). Hence \( \Phi_{\tilde{k}=0} \) has the same sign as \( h_x \) thus also the expectation value \( \sum_{\tilde{k}} \langle \Phi_{\tilde{k}} \sigma^x \Phi_{\tilde{k}} \rangle \) from the finite \( \tilde{k} \) modes. We sketch the expected behavior in Fig. 2. We have not yet developed a theory for \( T < T_c \).

III. CONCLUSIONS

In this paper, we examine carefully the condition of vestigial nematic order for a nematic superconductor. While the nematic superconducting ground state is expected for \( -\beta_1 < \beta_2 < 0 \), only the “deeper” part of this region with \( -\beta_1 < \beta_2 < -\beta_1/2 \) (\( g_2 > 0 \)) can exhibit vestigial nematic order above the superconducting state. The interpretation of the experiment \( 18 \), if correct, would exclude a large region of parameter space. Conversely, if the microscopic theory can constraint these parameters to the alternate region, then a different interpretation of the results in \( 18 \) must be sought. \( \beta_{1,2} \) in particular depend on the momentum and spin structure of the order parameter, and many model calculations have been given in the literature \( 14, 36-38 \). In \( 14 \), two models are studied, but both of them have \( g_2 > 0 \). Refs. \( 11, 36, 38 \), plotted phase diagrams containing both nematic and chiral phases, but they did not indicate explicitly the positions corresponding to \( g_2 = 0 \). However, since large regions of their nematic phases actually border the chiral phase, we know at least that those regions cannot exhibit vestigial nematic order. \( 36 \)

We remark that this is not the only example where a nematic superconductor behaves qualitatively differently according to the parameters \( \beta \)'s. Previously, when investigating the stability of half-quantum vortices near the lower critical field \( 15 \), we found that they are always stable for \( g_2 > 0 \). On the other hand, two half-quantum vortices might “collapse” back to an ordinary phase vor-
if the transition were second order. 

contribute, and the last term in eq (A1) vanishes after tex if \( g_2 < 0 \), unless counter-balanced by sufficiently large \( K_{23} \). Thus to understand the properties of a nematic superconductor and thus doped Bi2Se3, it is crucial to discern in which parameter region the system lies, and whether and how this depends on parameters such as doping concentrations.

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Appendix A: Nematic Susceptibility

Here we want to verify the condition \( g_2 < 0 \) for vestigial nematic order by evaluating the “nematic susceptibility”, in particular we would like to check that this is not an artifact of the particular basis we have chosen. We thus now use the original \( \eta \) notation, thus Hamiltonian eq \( \text{(5)} \) and \( \text{(7)} \). We evaluate the susceptibility to an external field coupling to \( \eta^i \tau_x \eta \) with zero external momentum. This susceptibility, in the random phase approximation, is given by the product of two Green’s function with an external vertex \( \tau_x \) and a renormalized vertex \( \Gamma^{(z)} \), which is given by the Bethe-Salpeter equation

\[
\Gamma^{(z)}_{ij} = \langle \Phi^i \Phi^j \rangle - \beta_1 \delta_{ij} T \sum_{\vec{k}} \left[ G_{i1l}(\vec{k}) \Gamma^{(z)}_{l1} G_{l1}(\vec{k}) \right] - \beta_1 T \sum_{\vec{k}} \left[ G_{i1l}(\vec{k}) \Gamma^{(z)}_{l1} G_{l1}(\vec{k}) \right] \\
- \beta_2 T \sum_{\vec{k}} \left[ \tau^\mu_{ij} G(\vec{k}) G_{l1l}(\vec{k}) \Gamma^{(z)}_{il1} G_{l1l}(\vec{k}) \right] - \beta_2 T \sum_{\vec{k}} \left[ \tau^\mu_{ij} G(\vec{k}) G_{l1l}(\vec{k}) \Gamma^{(z)}_{il1} G_{l1l}(\vec{k}) \right]
\]

(A1)

where \( i, j \) runs over the two components in \( \eta \) space and \( \mu = x, z \), here \( G \) is the Green’s function for \( \eta \) in zero field, that is \( G(\vec{k}) = \frac{\sin(k_a \tau_x)}{\sin(\frac{\pi}{2} \tau_x)} \) (c.f. eq \( \text{(7)} \)). One can check that \( \Gamma^{(z)} \) is proportional to \( \tau_x \), so let us denote this coefficient by \( \Gamma^{(z)} \). It is convenient to write \( G = G_0 + G_x \tau_x + G_z \tau_z \).

With this, we see that the first interacting term does not contribute, and the last term in eq \( \text{(A1)} \) vanishes after sum over \( \mu \), and we obtain the self-consistent equation

\[
\Gamma^{(z)} = 1 - (\beta_1 + 2\beta_2) T \sum_{\vec{k}} \left[ G_0 G_0 - G_x G_x + G_z G_z \right] \Gamma^{(z)}
\]

(A2)

where we have left out the arguments \( (\vec{k}) \) of \( G_0 \) etc for simplicity. Since the sums \( \sum_{\vec{k}} (G_x G_x) \) and \( \sum_{\vec{k}} (G_z G_z) \)
are equal, we get

\[ \Gamma^x(x) = \left[ 1 + (\beta_1 + 2\beta_2)T \sum_{E} (G_0 G_0) \right]^{-1} \]  

(A3)

Hence the vertex \( \Gamma^x(x) \) and the susceptibility diverges at

\[ 1 + g_2 T \sum_{\ell} \frac{(\alpha + \epsilon_0)^2}{D_0^2} = 0 \]  

(A4)

This is possible only if \( g_2 < 0 \), and in that case, eq (A4) is the same condition as \( \alpha = 0 \). Note that, using (24) a of eq (25) can also be rewritten as \( \alpha = -T \sum_{\ell} \frac{(\alpha + \epsilon_0)^2}{D_0^2} \).

We obtain exactly the same criterion if we consider the response to \( \tau^z \). In the above we have evaluated the nematic susceptibility for an non-interacting system. If we insert one-loop self-energies to the propagators, we would only modify the \( \alpha \)'s in \( \mathbf{G}(\mathbf{k}) \) to \( \alpha + (2g_1 + g_2)T \sum_{\ell} G_0(\mathbf{k}) \).

This just replaces these \( \alpha \)'s by the effective ones and thus does not affect the requirement that \( g_2 \) has to be negative for the divergence of the nematic susceptibility.

Appendix B: Mathematical Details and Further Estimates

We first consider some symmetry properties. Under a \( 2\pi/3 \) rotation, we map \((k_x, k_y)\) to \((k'_x, k'_y) = (ck_x - sk_y, sk_x + ck_y)\) with \( c = \cos(2\pi/3) \) and \( s = \sin(2\pi/3) \). Correspondingly \( k_x \pm ik_y \to (k_x \pm ik_y)\omega^{\pm 1} \) where \( \omega \equiv e^{2\pi i/3} \). Since \( \Phi_{1,4} \propto (\eta_x \pm i\eta_y) \), we have \( \Phi_{1,4} \to \Phi_{1,4}\omega^{\pm 1} \). Also \( G_{1,4} \to \omega^{-1}G_{1,4} \), corresponding \( (h_x \pm i\eta_y) \to (h_x \pm i\eta_y)\omega^{\pm 1} \).

The symmetry property of \( \epsilon_x \pm i\epsilon_y \) follows from that of \((k_x \pm ik_y)\) (note the negative sign in the definition of \( \epsilon_y \)): \( \epsilon_x \pm i\epsilon_y \to (\epsilon_x \pm i\epsilon_y)\omega^{\pm 1} \). Hence \( \epsilon \) transform in the same manner as \( \bar{h} \), with the two components transforming as \((k_x^2 - k_y^2, -2k_xk_y)\) under \( D_{3d} \).

For the momentum sums, we note that \( D_0 \) is an invariant. It follows immediately that sums of the form \( \sum_{\ell} \frac{(\epsilon_0)^2}{D_0^2} \) vanish unless \( j \) is a multiple of 3. From these we see that \( \sum_{\ell} \frac{(\epsilon_0)^2}{D_0^2} = \sum_{\ell} \frac{\epsilon_0^2}{D_0^2} = 0 \), whereas \( \sum_{\ell} \frac{(\epsilon_0)^2}{D_0^2} = \sum_{\ell} \frac{\epsilon_0^2}{D_0^2} \).

Also, using the transformation property of \( \epsilon_{x,y} \), we obtain \( \sum_{\ell} \frac{\epsilon_0^2}{D_0^2} = -\sum_{\ell} \frac{\epsilon_0^2}{D_0^2} \), and \( \sum_{\ell} \frac{\epsilon_0^2}{D_0^2} = 3 \sum_{\ell} \frac{(\epsilon_0)^2}{D_0^2} \).

We now turn to the evaluation of some of the sums and integrals.

Let us consider a of eq (26), and approximate the denominator \( D_0 \) there by \( D_{00} \) as discussed in text. That is, we would like to calculate the sum \(-T \sum_{\ell} \frac{\epsilon_0^2}{D_{00}} \). To do this, we introduce \( x = \left( \frac{K}{\alpha} \right)^{1/2} k_x \) and similarly for \( x \to y \) and \( z = \left( \frac{K}{\alpha} \right)^{1/2} k_z \). This sum then becomes

\[ -T \frac{\alpha^{3/2}}{K} \frac{1}{K^{1/2} \alpha^2} \int \frac{d^2x}{(2\pi)^3} \frac{1}{1 + R^2} \]  

(B1)

where \( R^2 \equiv (x^2 + y^2 + z^2) \). The integral gives \( 1/(8\pi) \) hence eq (10). The terms in eq (83) and (89) are obtained in similar manner.

Let us examine the second contribution to a in eq (25). That is, \(-T \sum_{\ell} \frac{\epsilon_0^2}{D_0} \). Similar to above, we first replace the denominator \( D_0 \) there by \( D_{00} \) and use the same substitutions as above. After this we can replace \((x^2 - y^2)^2\) etc by their angular averages. We obtain the contribution

\[ -T \frac{\alpha^{3/2}}{K} \frac{1}{K^{1/2} \alpha^2} \left[ \frac{(K_{23})^2}{K} + \frac{(K')^2}{K_{23}K} \right] \frac{2}{15} \int \frac{d^3x}{(2\pi)^3} \frac{R^4}{(1 + R^2)^4} \]  

(B2)

The factor \( 2/15 \) is from the angular average. Note that the last term has the same large \( R \) dependence as eq (131) but has higher \( R \) powers at \( R \to 0 \). The integral gives \( 5/(26\pi) \). Hence this contribution is much smaller than the one given in (131) even when the quantity in the square bracket of eq (132) is of order 1. (The correction is \( \frac{1}{15} \times \frac{2}{2\pi} \times 8\pi = \frac{1}{12} \) of the original). This is because of (i) the angular average and (ii) the smaller \( d^3x \) integral, which is in turn due to the higher powers in \( R \) arising from the \( \epsilon^2 \) factor.

Similar remarks apply to the other terms in, e.g., eq (24) and (30). Note also that, when we restore the \( \epsilon^2 \) in the denominators \( D_0 \) but expand in it, the correction terms are exactly of the same forms as the “higher order”
terms in these equations. Hence we conclude that, unless in extreme circumstances of very large $K_{23}$ compared with $\tilde{K}$ etc, the condition for $\bar{c} > 0$ is, to a good approximation, given as in text. (Gradient terms were evaluated in, e.g.,[14] for two models, giving $K_{23}/\tilde{K} = 1$ and $2/3$; $K'$ was not given there) Note also that the condition $\epsilon_0^2 > \epsilon^8$ limit the sizes of $K_{23}/\tilde{K}$ and $K'^2/(\tilde{K}K_{zz})$. That is, unless the system is close to one where the net gradient energy is small along some momentum directions, the stability condition we gave is a good approximation.

Now let us turn to $b$ in eq (20). Replacing $\tilde{K}$ by $x, y, z$ as explained above, the sum $\sum_k \frac{\partial^3 \epsilon}{\partial \phi}^2$ becomes

$$\frac{1}{4} \frac{\alpha^{3/2}}{K} \frac{1}{K^{1/2} \alpha^3} \int \frac{d^3 \phi}{(2\pi)^3} \left[ (\delta^3 \cos(6\phi) - 3\delta^2 \kappa_1 \sin(3\phi) - \kappa^3 /\tilde{K} \sin(3\phi)) \right]$$

where $\delta \equiv (K_{23}/K)$ and $\kappa = K'/K(K_{zz} \tilde{K})^{1/2}$, and we have defined $r$ and $\phi$ by $(x, y) = r(\cos(\phi), \sin(\phi))$. We have also dropped terms such as $\sin(\phi)$ and $\cos(\phi)$ in the numerator which vanish after integration. We see that $b$ is finite only when $K_{23}$ and $K'$ are both finite, and for small $K_{23}$ and $K'$, proportional to $K_{zz}^2 K'^2$. Thus $b$ vanishes if the system has $D_{hh}$ symmetry. In the same spirit as the approximations taken above, the parametric dependences of $b$ can be estimated as

$$b \sim -T \frac{\alpha^{3/2}}{K} \frac{1}{K^{1/2} \alpha^3} \left( \frac{K_{23}}{K} \right)^3 (K')^2 K_{zz}$$

For simplicity of the presentation, we shall not display the numerical coefficient, which is found to be $33/(4 \times 4096 \pi)$. This small coefficient is again due to the angular averages and high powers of $k$’s in the numerator of eq (20), similar to what we have encountered in the estimation eq (19) for the second contribution to $a$. Correspondingly,

$$\frac{g_2 b^2}{c'} \sim \frac{g_2}{2g_1 + g_2} \left( \frac{K_{23}}{K} \right)^3 (K')^2 \left( \frac{K_{zz}}{K} \right)$$

Thus $g_2 b^2$ is expected to give only a small contribution to $\bar{c}$, especially if $g_2$ is small compared with $g_1$ or when $K'$ is small etc.

We now estimate $|\tilde{b}|$ at the first order transition at $T_1^*$ and compare it with $\alpha(T_1^*)$. We first note that $\alpha(T_1^*) > \alpha(T_1)$ since $T_1^* > T_1$ using eq (13) and (39) and (40), we get

$$\frac{|\tilde{b}|}{c' \alpha(T_1^*)} \sim \frac{|g_2|}{2g_1 + g_2} \left( \frac{K_{23}}{K} \right)^3 (K')^2 \left( \frac{K_{zz}}{K} \right)$$

with an expectation small numerical factors implicit. If we consider $|b|/|\tilde{b}(T_1)|$, instead then a generous estimate would be to replace the term $(2g_1 + g_2)$ by $(2g_1 - |\tilde{b}|/2g_2)$ as explained below eq (11). Hence unless $|g_2| \approx g_1$ and with very special circumstances for the gradient coefficients, we have $\alpha > |\tilde{b}|$ at $T_1^*$, and the superconducting order parameter nucleates only at a lower temperature, as sketched in Fig. 2.

Lastly we estimate $T_1^* - T_1$. This is

$$T_1^* - T_1 \approx \frac{b^2}{c} \left( \frac{\partial a}{\partial T} \right)$$

Note that $\frac{\partial a}{\partial T} = \frac{\partial a}{\partial T}$. If we again replace $\bar{c}$ by $c'$, we get the estimate

$$T_1^* - T_1 \sim \frac{|g_2|}{(2g_1 + g_2)} \left( \frac{|g_2|}{\alpha' K^2 K_{zz}} \right)$$

with a small coefficient due to $b$ implicit. Note again the appearance of a Ginzburg-like parameter on the right and compare this with eq (11).

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[35] The fact that $\text{sgn} h_2$ is independent of $\text{sgn} K'$ can be understood as follows. A crystal with $D_{3d}$ has no $z \to -z$ reflection symmetry. Under this reflection, the original crystal would turn into a new one with $K_{23}$ remaining the same whereas $K'$ changes sign. Under this reflection however, the direction of the vestigial order (which is related to an in-plane distortion) hence $h_2$ does not change.

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[24] This condition is necessary but not sufficient. For additional discussions, see, e.g., \[22\]