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Vortices with magnetic field inversion in non-centrosymmetric superconductors

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Superconducting materials with non-centrosymmetric lattices lacking the space inversion symmetry exhibit a variety of interesting parity-breaking phenomena, including magneto-electric effect, spin-polarized currents, helical states, and unusual Josephson effect. We demonstrate, within a Ginzburg-Landau framework describing non-centrosymmetric superconductors with O point group symmetry, that vortices can exhibit an inversion of the magnetic field at a certain distance from the vortex core. In a stark contrast to conventional superconducting vortices, the magnetic-field reversal in the parity-broken superconductor leads to non-monotonic intervortex forces and, as a consequence, to the exotic properties of the vortex matter such as the formation of vortex bound states, vortex clusters, and appearance of metastable vortex/anti-vortex bound states.

I. INTRODUCTION

Non-centrosymmetric superconductors are superconducting materials whose crystal structure is not symmetric under the spatial inversion. These parity-breaking materials have attracted much theoretical [1, 2] and experimental [3–5] interest, as they open the possibility to investigate spontaneous breaking of a continuous symmetry in a parity-violating medium (for recent reviews, see [6–8]). The parity-breaking nature of the superconducting order parameter [4, 5] in the non-centrosymmetric superconductors leads to various unusual magnetoelectric phenomena due to the mixing of singlet and triplet components of the superconducting condensate, correlations between supercurrents and spin polarization, to the existence of helical states, and unusual structure of vortex lattices.

Moreover, parity breaking in the non-centrosymmetric superconductors also results in an unconventional Josephson effect, where the junction features a phase-shifted relation for the Josephson current [9, 10]. Unconventional Josephson junctions consisting of two non-centrosymmetric superconductors linked by a uniaxial ferromagnet were recently proposed as the element of a qubit that avoids the use of an offset magnetic flux, enabling a simpler and more robust architecture [11].

In the macroscopic description of such superconducting states, the lack of inversion symmetry yields new terms in the Ginzburg-Landau free energy represented by the so-called the Lifshitz invariants. These terms directly couple the magnetic field \mathbf{B} to the supercurrent \mathbf{j} and thus lead to a variety of new effects that are absent in conventional superconductors. The explicit form of the allowed Lifshitz invariant depends on the point symmetry group of the underlying crystal structure.

In this paper, we consider a particular class of non-centrosymmetric superconductors whose macroscopic interactions break the discrete group of parity reversals

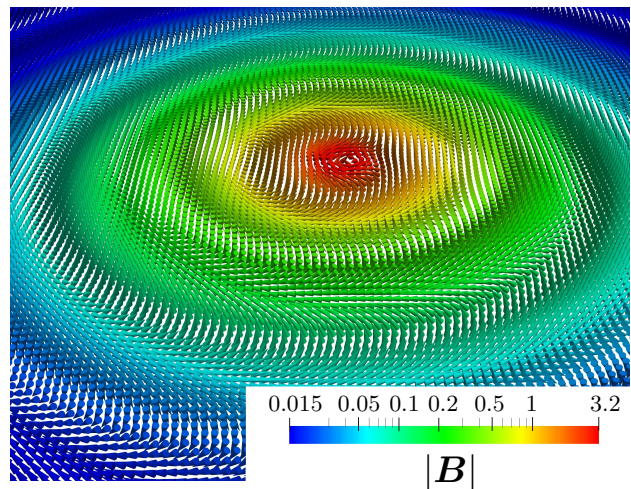


Figure 1. Inversion patterns of the magnetic field \mathbf{B} of a vortex in a non-centrosymmetric superconductor. The magnetic field forms helicoidal patterns around a straight static vortex. As the distance from the vortex core increases, the longitudinal (parallel to the vortex core) component of the magnetic field may change its sign. The magnetic field may exhibit several sign reversals in the normal plane. In the picture, which is a result of a numerical simulation of the Ginzburg-Landau theory, the colors encode the amplitude of the magnetic field \mathbf{B} , in a normal plane with respect to the vortex line while the arrows demonstrate the orientation of the field.

and, at the same time, are invariant under spatial rotations. The corresponding Lifshitz invariant featuring these symmetries is described by a simple, parity-violating isotropic term, $\gamma \mathbf{j} \cdot \mathbf{B}$, where the coupling γ determines the strength of the parity breaking. This particular structure describes non-centrosymmetric superconductors with O point group symmetry such as $\text{Li}_2\text{Pt}_3\text{B}$ [5, 12], $\text{Mo}_3\text{Al}_2\text{C}$ [13, 14], and PtSbS [15].

Vortex states in cubic non-centrosymmetric supercon-

ductors feature a transverse magnetic field, in addition to the ordinary longitudinal field. Consequently, they also carry a longitudinal current on top of the usual transverse screening currents [16–18]. Therefore, as illustrated in Fig. 1, both the superconducting current and the magnetic field form a helical-like structure that winds around the vortex core (for additional material illustrating the helical spatial structure of the magnetic streamlines, see Appendix B, and animations [19]). The previous theoretical papers studied vortices in the perturbative regime where the coupling to the Lifshitz invariant γ is small, either in the London limit (with a large Ginzburg-Landau parameter) [16, 17], or beyond it [18]. For currently known non-centrosymmetric materials, these approximations are valid since the magnitude of the Lifshitz invariants, which can be estimated in a weak-coupling approximation, is typically small. We propose here a general study of vortices, for all possible values of the Lifshitz invariant coupling, both in the London limit and beyond.

We demonstrate that vortices may feature an inversion of the magnetic field at distance of about $4\lambda_L$ from the vortex center. Moreover, for rather high values of the coupling γ , alternating reversals may occur several times, at different distances from the vortex core. Such an inversion of the magnetic field is illustrated, in Fig. 1. The reversal of the magnetic field, which is in stark contrast to conventional superconducting vortices, becomes increasingly important for larger couplings of the Lifshitz invariant term. This property of field inversion is responsible for other unusual behaviours, also absent in conventional type-2 superconductors. Indeed, we show that it leads to the formation of vortex bound states, vortex clusters, and meta-stable pairs of vortex and anti-vortex. These phenomena should have numerous physical consequences on the response of non-centrosymmetric superconductors to an external magnetic field.

The paper is organized as follows. In Sec. II, we introduce the phenomenological Ginzburg-Landau theory that describes the superconducting state of a non-centrosymmetric material with the O point group symmetry. Next, in Sec. III we investigate the properties of single vortices both in the London limit and beyond it. We also demonstrate that the parity-breaking superconductors can feature an inversion of the longitudinal magnetic field. This observation suggests that the intervortex interaction in parity-odd superconductors might be much richer than that for a conventional superconductor. Hence we derive analytically the intervortex interaction energy in the London limit in Sec. IV. We show that the interaction potential depends non-monotonically on the intervortex distance, which leads to the existence of vortex bound states. Using numerical minimization of the Ginzburg-Landau free energy, we further observe that such bound states persist beyond the London limit. Our conclusions and discussion of further prospects are given in the last section.

II. THEORETICAL FRAMEWORK

We consider non-centrosymmetric superconductors with the crystal structure possessing the O point group symmetry. Such materials are described, in the vicinity of the superconducting critical temperature, by the Ginzburg-Landau free energy $F = \int d^3x \mathcal{F}$ with the free-energy density given by (see e.g. [6, 20]):

$$\mathcal{F} = \frac{\mathbf{B}^2}{8\pi} + k|\mathbf{D}\psi|^2 + \gamma\mathbf{j} \cdot \mathbf{B} + \frac{\beta}{2}(|\psi|^2 - \psi_0^2)^2, \quad (1)$$

where $\mathbf{j} = 2e \text{Im}(\psi^* \mathbf{D}\psi)$; we use $\hbar=c=1$. Here, the single component order parameter $\psi = |\psi|e^{i\varphi}$ is a complex scalar field that is coupled to the vector potential \mathbf{A} of the magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$ through the gauge derivative $\mathbf{D} \equiv \nabla - ie\mathbf{A}$, where e is a gauge coupling. The explicit breaking of the inversion symmetry is accounted by the Lifshitz invariant term with the prefactor γ , that directly couples the magnetic field \mathbf{B} and the supercurrent $\mathbf{j} = 2e|\psi|^2(\nabla\varphi - e\mathbf{A})$. The current \mathbf{j} is the usual superconducting current at $\gamma = 0$, i.e. in the absence of parity breaking. The parameter γ can be chosen to be positive without loss of generality. At a nonzero parity-breaking coupling γ , the current gets an additional contribution from the Lifshitz term [20]. The other coupling constants k and β describe, respectively, the magnitude of the kinetic and potential terms in the free energy (1).

The variation of the free energy (1) with respect to the scalar field ψ^* yields the Ginzburg-Landau equation for the superconducting condensate,

$$[k\mathbf{D} + 2ie\gamma\mathbf{B}] \cdot \mathbf{D}\psi = \beta(|\psi|^2 - \psi_0^2)\psi, \quad (2)$$

while the variation of the free energy with respect to the gauge potential \mathbf{A} gives the Ampère-Maxwell equation:

$$\nabla \times \left(\frac{\mathbf{B}}{4\pi} + \gamma\mathbf{j} \right) = k\mathbf{j} + 2\gamma e^2 |\psi|^2 \mathbf{B}. \quad (3)$$

The physical length scales of the theory are the coherence length ξ and the London penetration depth λ_L ,

$$\xi^2 = \frac{k}{2\beta\psi_0}, \quad \text{and} \quad \lambda_L^2 = \frac{1}{8\pi k e^2 \psi_0^2}, \quad (4)$$

respectively. The Ginzburg-Landau parameter, $\kappa = \lambda_L/\xi$, is given by the ratio of these characteristic length scales.

Note that since the parity-violating term in the Ginzburg-Landau model (1) is not positively defined, the strength of the parity violation cannot be arbitrarily large. For the free energy to be bounded from below in the ground state, the parity-odd parameter γ cannot exceed a critical value,

$$0 \leq \gamma < \gamma_*, \quad \text{where} \quad \gamma_* = \sqrt{\frac{k}{8\pi e^2 \psi_0^2}} = k\lambda_L. \quad (5)$$

A detailed discussion of the positive definiteness, and the derivation of the range of validity are given in Appendix A. The bound (5) implies that the parity breaking

should not be too strong in order to ensure the validity of the minimalistic Ginzburg-Landau model (1). Note however that the upper bound on the parity-violating coupling applies only to the form of the free energy functional (1). If the parity violating coupling γ exceeds the critical value (5), the model has to be supplemented with higher-order gradient terms, for the energy to be bounded.

III. VORTICES IN NON-CENTROSYMMETRIC SUPERCONDUCTORS

Vortices are the elementary topological excitations in superconductors. Below, in the London limit, we derive vortex solutions for any values of the coupling $\gamma < \gamma_*$. As previously stated, the new solutions described here exhibit very unusual properties like the inversion of the magnetic field, which allows for the vortex bound states formation. While this property is interesting by itself, it is also important to verify that the overall physical picture advocated here is not merely an artifact of the London limit. Consequently, we check that the results obtained in the London limit are consistent with the numerical solutions of the full nonlinear problem, by using the following procedure.

The Lifshitz invariant is a scalar under rotations, thus solutions are the same for any orientation of the surface normal. It thus makes sense to consider the case of field configurations that are translationally invariant along the z -axis. Thus, the fields should respect symmetries generated by the Killing vector $K_{(z)} = \partial/\partial z$. Since all internal symmetries of the theory are gauged, there exist a gauge where the fields do not depend on z [21]. A reasonable field ansatz is thus

$$\mathbf{A} = (A_x(x, y), A_y(x, y), A_z(x, y)) \text{ and } \psi = \psi(x, y). \quad (6)$$

To investigate the properties of the vortex solutions, the physical degrees of freedom ψ and \mathbf{A} are discretized within a finite-element formulation [22], and the Ginzburg-Landau free energy (1) is subsequently minimized using a non-linear conjugate gradient algorithm. Given a starting configuration where the condensate has a specified phase winding (at large distances $\psi \propto e^{i\theta}$ and θ is the polar angle relative to the vortex center), the minimization procedure leads, after convergence of the algorithm, to the vortex solution of the full nonlinear theory [23].

A. London limit solutions

In the London limit, $\kappa \rightarrow \infty$, the superconducting condensate is approximated to have a constant density, $|\psi| = \psi_0$. Hence the supercurrent now reads as $\mathbf{j} = 2e\psi_0^2 (\nabla\varphi - e\mathbf{A})$. It leads to the second London equation that relates the magnetic field and the super-

current

$$\mathbf{B} = \frac{1}{e} \left(\nabla \times \nabla\varphi - \frac{1}{2e\psi_0^2} \nabla \times \mathbf{j} \right). \quad (7)$$

The constant density approximation, together with Eq. (7), is then used to rewrite the the Ampère-Maxwell equation (3) as the London equation for the current:

$$\lambda_L^2 \nabla \times \nabla \times \mathbf{j} + \mathbf{j} - 2\frac{\gamma}{k} \nabla \times \mathbf{j} = S, \quad (8)$$

where the source term on the right hand side,

$$\begin{aligned} S &= \frac{1}{4\pi k e} \left(\nabla \times \nabla \times \nabla\varphi - \frac{\gamma}{k\lambda_L^2} \nabla \times \nabla\varphi \right) \\ &= \frac{\Phi_0}{4\pi k} \left(\nabla \times \mathbf{v} - \frac{\gamma}{k\lambda_L^2} \mathbf{v} \right), \text{ with } \mathbf{v} = \frac{1}{2\pi} \nabla \times \nabla\varphi. \end{aligned} \quad (9)$$

Here $\Phi_0 = 2\pi/e$ is the elementary flux quantum, and \mathbf{v} is the density of vortex field that accounts for the phase singularities.

In the dimensionless units, $\tilde{\mathbf{x}} = \frac{\mathbf{x}}{\lambda_L}$, $\tilde{\nabla} = \lambda_L \nabla$, the London equation is

$$\begin{aligned} \tilde{\nabla} \times \tilde{\nabla} \times \mathbf{j} + \mathbf{j} - 2\Gamma \tilde{\nabla} \times \mathbf{j} &= \frac{\Phi_0}{4\pi k \lambda_L} \left(\tilde{\nabla} \times \mathbf{v} - \Gamma \mathbf{v} \right) \\ \text{and } \mathbf{B}(\tilde{\mathbf{x}}) &= \Phi_0 \mathbf{v} - 4\pi k \lambda_L \tilde{\nabla} \times \mathbf{j}. \end{aligned} \quad (10)$$

For the energy to be bounded, the criterion (5) implies that the dimensionless coupling $\Gamma = \gamma/k\lambda_L$ introduced here, satisfies $0 \leq \Gamma < 1$. Defining the amplitude $\mathcal{A} = \frac{\Phi_0}{4\pi k \lambda_L}$, the momentum space London equation reads as

$$\begin{aligned} -\mathbf{p} \times \mathbf{p} \times \mathbf{j}_{\mathbf{p}} + \mathbf{j}_{\mathbf{p}} - 2i\Gamma \mathbf{p} \times \mathbf{j}_{\mathbf{p}} &= \mathcal{A} \left(i\mathbf{p} \times \mathbf{v}_{\mathbf{p}} - \Gamma \mathbf{v}_{\mathbf{p}} \right), \\ \text{and } \mathbf{B}_{\mathbf{p}} &= \Phi_0 \mathbf{v} - 4\pi i k \lambda_L \mathbf{p} \times \mathbf{j}_{\mathbf{p}}. \end{aligned} \quad (11)$$

where $\mathbf{j}_{\mathbf{p}}$ is the Fourier component of the current \mathbf{j} in the space of the dimensionless momenta \mathbf{p} :

$$\mathbf{j}(\tilde{\mathbf{x}}) = \int \frac{d^3\mathbf{p}}{(2\pi)^3} e^{i\mathbf{p}\cdot\tilde{\mathbf{x}}} \mathbf{j}_{\mathbf{p}}. \quad (12)$$

Similarly, the quantities $\mathbf{v}_{\mathbf{p}}$ and $\mathbf{B}_{\mathbf{p}}$ are, respectively, the Fourier components of $\mathbf{v}(\tilde{\mathbf{x}})$ and $\mathbf{B}(\tilde{\mathbf{x}})$. The solution of the algebraic equation (11) in the momentum space is

$$\begin{aligned} \mathbf{j}_{\mathbf{p}}^m &= \frac{\mathcal{A}}{\Sigma} \left\{ -\Gamma [(1 - \mathbf{p}^2)\delta_{mn} + (\Omega + 2)p^m p^n] \right. \\ &\quad \left. + i(\Omega + 2\Gamma^2)\epsilon_{mln} p^l \right\} v_{\mathbf{p}}^n := \Phi_0 \Lambda_{\mathbf{p}}^{mn} v_{\mathbf{p}}^n, \end{aligned} \quad (13)$$

$$\begin{aligned} \mathbf{B}_{\mathbf{p}}^m &= \frac{\Phi_0}{\Sigma} \left\{ [1 + (1 - 2\Gamma^2)\mathbf{p}^2]\delta_{mn} + (\Omega + 2\Gamma^2)p^m p^n \right. \\ &\quad \left. + i\Gamma(1 - \mathbf{p}^2)\epsilon_{mln} p^l \right\} v_{\mathbf{p}}^n := \Phi_0 \Upsilon_{\mathbf{p}}^{mn} v_{\mathbf{p}}^n, \end{aligned} \quad (14)$$

with the polynomials $\Sigma \equiv \Sigma(\mathbf{p}^2) = (1 + \mathbf{p}^2)^2 - 4\Gamma^2 \mathbf{p}^2$ and $\Omega \equiv \Omega(\mathbf{p}^2) = 1 + \mathbf{p}^2 - 4\Gamma^2$. Here δ_{mn} and ϵ_{mln} are, respectively, the Kronecker and the Levi-Civita symbols, and the silent indices are summed over.

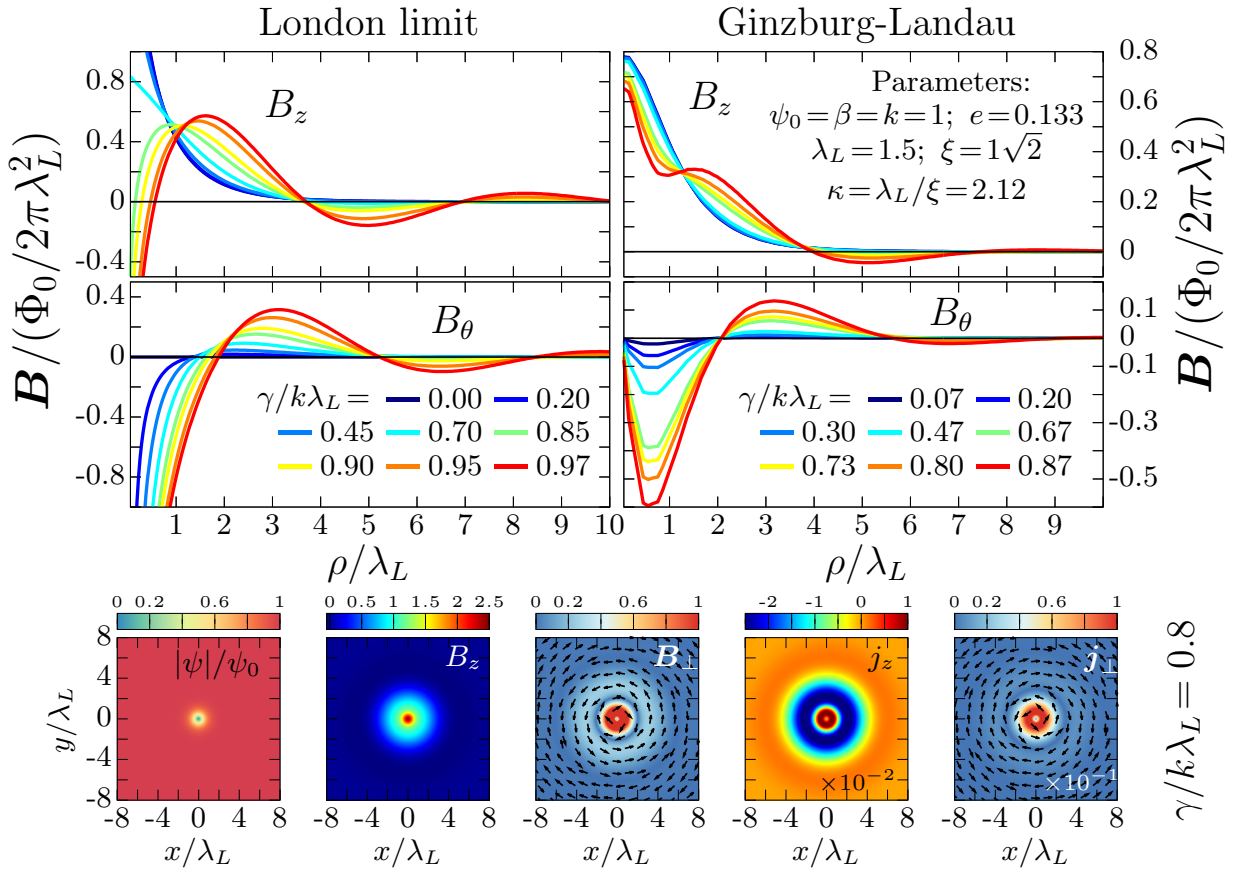


Figure 2. The upper row displays the longitudinal (B_z) and circular (B_θ) components of the magnetic field of a single vortex, as functions of the radial distance ρ from the vortex center for various values of the parity-odd coupling γ . The left and right panels show the magnetic field in the London limit and beyond the London approximation, respectively. The panels in the bottom row, result from the minimization of the Ginzburg-Landau free energy at the parity-breaking coupling $\gamma = 0.8\gamma_*$. They show the superconducting condensate $|\psi|$, the longitudinal and transverse components of the magnetic field, B_z and \mathbf{B}_\perp , and supercurrents, j_z and \mathbf{j}_\perp , in the transverse plane of the vortex. In the case of a weak parity violation, $\gamma \ll \gamma_*$, the longitudinal component of the magnetic field is similar to that of conventional Abrikosov vortices for which $B_z(\rho)$ is monotonic and exponentially localized at the vortex core at $\rho = 0$. When the parity-breaking term becomes large, with γ approaching the critical value γ_* , the longitudinal component B_z becomes a non-monotonic function as the distance ρ from the vortex core increases.

Thus, the vortex field \mathbf{v} completely determines, via its Fourier image $\mathbf{v}_\mathbf{p}$, the momentum-space representations of the supercurrent (13) and of the magnetic field (14). The corresponding real space solutions are obtained by the Fourier transformation (12). Assuming the translation invariance along z -axis, a set of N vortices located at the positions $\tilde{\mathbf{x}}_a$, and characterized by the individual winding numbers n_a (with $a = 1, \dots, N$), is described by the Fourier components

$$\mathbf{v}_\mathbf{p} = 2\pi \frac{\delta(p_z) \mathbf{e}_z}{\lambda_L^2} \sum_{a=1}^N n_a e^{-i\mathbf{p} \cdot \tilde{\mathbf{x}}_a}, \quad (15)$$

where the Dirac delta for the momentum p_z specifies the translation invariance of the configuration.

B. Single vortex

The analysis becomes particularly simple for a single elementary vortex with a unit winding number ($n_1 = 1$) located at the origin ($\mathbf{x}_1 = 0$). The corresponding magnetic field reads as follows:

$$\mathbf{B}_\mathbf{p} = \frac{2\pi\Phi_0\delta(p_z)}{\lambda_L^2\Sigma} \begin{pmatrix} i\Gamma(1-\mathbf{p}^2)p_y \\ -i\Gamma(1-\mathbf{p}^2)p_x \\ (1-2\Gamma^2)\mathbf{p}^2 + 1 \end{pmatrix}. \quad (16)$$

Next, we express the position, $\tilde{\mathbf{x}} = (\tilde{\rho} \cos \theta, \tilde{\rho} \sin \theta, \tilde{z})$, and momentum, $\mathbf{p} = (q \cos \vartheta, q \sin \vartheta, p_z)$, in cylindrical coordinates. An integration over the angular degrees of freedom ϑ nullifies the radial part B_ρ of the magnetic field and generates the Bessel functions of the first kind, J_0 and J_1 . Hence, the nonzero components of the magnetic field can be expressed as one dimensional integrals over

the radial momentum q :

$$\begin{aligned} B_\theta\left(\frac{\rho}{\lambda_L}\right) &= \frac{\Phi_0\Gamma}{2\pi\lambda_L^2} \int_0^\infty \frac{q^2(1-q^2)dq}{(1+q^2)^2-4\Gamma^2q^2} J_1\left(\frac{q\rho}{\lambda_L}\right) \\ B_z\left(\frac{\rho}{\lambda_L}\right) &= \frac{\Phi_0}{2\pi\lambda_L^2} \int_0^\infty \frac{q[(1-2\Gamma^2)q^2+1]dq}{(1+q^2)^2-4\Gamma^2q^2} J_0\left(\frac{q\rho}{\lambda_L}\right). \end{aligned} \quad (17)$$

Similarly, the nonzero components of the current are:

$$\begin{aligned} j_\theta\left(\frac{\rho}{\lambda_L}\right) &= \frac{\Phi_0}{8\pi^2k\lambda_L^3} \int_0^\infty \frac{q^2(q^2+1-2\Gamma^2)dq}{(1+q^2)^2-4\Gamma^2q^2} J_1\left(\frac{q\rho}{\lambda_L}\right) \\ j_z\left(\frac{\rho}{\lambda_L}\right) &= \frac{-\Phi_0\Gamma}{8\pi^2k\lambda_L^3} \int_0^\infty \frac{q(1-q^2)dq}{(1+q^2)^2-4\Gamma^2q^2} J_0\left(\frac{q\rho}{\lambda_L}\right). \end{aligned} \quad (18)$$

In the absence of parity breaking, $\Gamma = 0$, these integrals can be solved analytically, in terms of the modified Bessel function of the second kind K_m . This expectedly gives the textbook expressions for the nonvanishing components of the magnetic field, $B_z(\rho/\lambda_L) = \frac{\Phi_0}{2\pi\lambda_L^2} K_0(\rho/\lambda_L)$, and of the superconducting current, $4\pi k j_\theta(\rho/\lambda_L) = \frac{\Phi_0}{2\pi\lambda_L^2} K_1(\rho/\lambda_L)$. The general case with a nonzero parity-breaking coupling, $\Gamma \neq 0$, requires a numerical evaluation of the integrals (17) and (18).

Figure 2 shows the magnetic field of a single vortex both in the London limit and for the full Ginzburg-Landau problem. First, although the solutions are expected to differ at the vortex core, the overall behaviour remains qualitatively similar in both cases. Indeed, the London solutions are divergent at the vortex core, and thus they require a sharp cut-off at the coherence length ξ . Solutions beyond the London limit, on the other hand, are regular everywhere. The bottom row of Fig. 2 shows a typical vortex solution obtained numerically beyond the London limit. This is a close-up view of the vortex core structure, while the actual numerical domain is much larger in order to prevent any finite size effect. While the density profile is similar to that of common vortices, the magnetic field shows a pretty unusual profile featuring a slight inversion, away from the center. For the current parameter set where $\gamma = 0.8\gamma_*$, the amplitude of the reversed field compared to the maximal amplitude is rather small. Yet, as illustrated on the top-right panels of Fig. 2, the amplitude of inversion of the magnetic field, typically increase with the parity-breaking coupling γ . Thus when γ is close to the critical coupling γ_* , the magnitude of the responses and field inversions become rather important.

When the parity-breaking coupling γ is small compared to the upper bound γ_* , the longitudinal component B_z of the magnetic field is monotonic and exponentially localized, as for conventional vortices. The vortex configurations start to deviate from the conventional case when the parity breaking strengthens. When γ approaches the critical value γ_* , the magnetic field B_z do not vary monotonically any longer. It can be reversed, and even feature several local minima as can be seen in the top-right panel of Fig. 2. Note that, the complicated spatial structure and inversion of the magnetic field also

comes with the inversion of the supercurrents. Note that the distance from the vortex center $\rho \simeq 4\lambda_L$ where the longitudinal component of the magnetic field first vanishes, corresponds to the radius where the in-plane current j_θ reverses its sign. Similarly, the longitudinal current j_z vanishes for the first time at the shorter distance to the vortex core, $\rho \simeq 2\lambda_L$, where the circular magnetic field cancels, $B_\theta = 0$. These observations are consistent with the results from the perturbative regime $\gamma \ll \gamma_*$ [18]. Interestingly, these specific radii are pretty much unaffected by the value of the parity-breaking coupling.

IV. VORTEX INTERACTIONS

The possibility of having an inversion of the magnetic field suggests that the interaction between two vortices might be much more involved than the pure repulsion that occurs in conventional type-2 superconductors. Indeed, since the conventional long-range intervortex repulsion is due to the magnetic field, it is quite likely that the interaction here might be not only quantitatively, but also qualitatively altered. To investigate these, we consider the London limit free energy F written in the previously used dimensionless coordinates. Using Eq. (12) to express the quantities \mathbf{j} and \mathbf{B} in terms of their Fourier components, yields the expression of the free energy in the momentum space:

$$\begin{aligned} F = \frac{\lambda_L^3}{8\pi} \int \frac{d^3\mathbf{p}}{(2\pi)^3} \left\{ \mathbf{B}_\mathbf{p} \cdot \mathbf{B}_{-\mathbf{p}} + (4\pi k\lambda_L \mathbf{j}_\mathbf{p}) \cdot (4\pi k\lambda_L \mathbf{j}_{-\mathbf{p}}) \right. \\ \left. + 2\Gamma(4\pi k\lambda_L \mathbf{j}_\mathbf{p}) \cdot \mathbf{B}_{-\mathbf{p}} \right\}. \end{aligned} \quad (19)$$

Replacing the Fourier components of the magnetic field $\mathbf{B}_\mathbf{p}$ and of the current $\mathbf{j}_\mathbf{p}$ with the corresponding expressions in terms of the vortex field $\mathbf{v}_\mathbf{p}$, Eqs. (13) and (14), respectively, yields the free energy:

$$F = \frac{\lambda_L^3}{8\pi} \int \frac{d^3\mathbf{p}}{(2\pi)^3} \mathbf{v}_\mathbf{p}^m G^{mn} \mathbf{v}_{-\mathbf{p}}^n \quad (20)$$

$$\text{where } G^{mn} = \Upsilon_\mathbf{p}^{lm} \Upsilon_{-\mathbf{p}}^{ln} + \Lambda_\mathbf{p}^{lm} \Lambda_{-\mathbf{p}}^{ln} + 2\Gamma \Lambda_\mathbf{p}^{lm} \Upsilon_{-\mathbf{p}}^{ln}.$$

The interaction matrix G has a rather involved structure. Yet, given that only the axial Fourier components of the vortex field (15) are nonzero, only the component G^{zz} will contribute to the energy. Up to terms that are proportional to p_z , and thus will be suppressed by the Dirac delta $\delta(p_z)$, G^{zz} takes the simple form

$$G^{zz} = \frac{(1-\Gamma^2)(1+\mathbf{p}^2)}{\Sigma} + \text{terms} \propto p_z. \quad (21)$$

Finally, using the vortex field ansatz (15), together with the expressions (21) and (20) determines the free energy associated with a set of translationally invariant vortices

$$F = \frac{\Phi_0^2(1-\Gamma^2)}{8\pi\lambda_L} \sum_{a,b=1}^N n_a n_b \int \frac{d^2\mathbf{p}}{2\pi} \frac{1+\mathbf{p}^2}{\Sigma(\mathbf{p}^2)} e^{i\mathbf{p}\cdot(\bar{\mathbf{x}}_a-\bar{\mathbf{x}}_b)}. \quad (22)$$

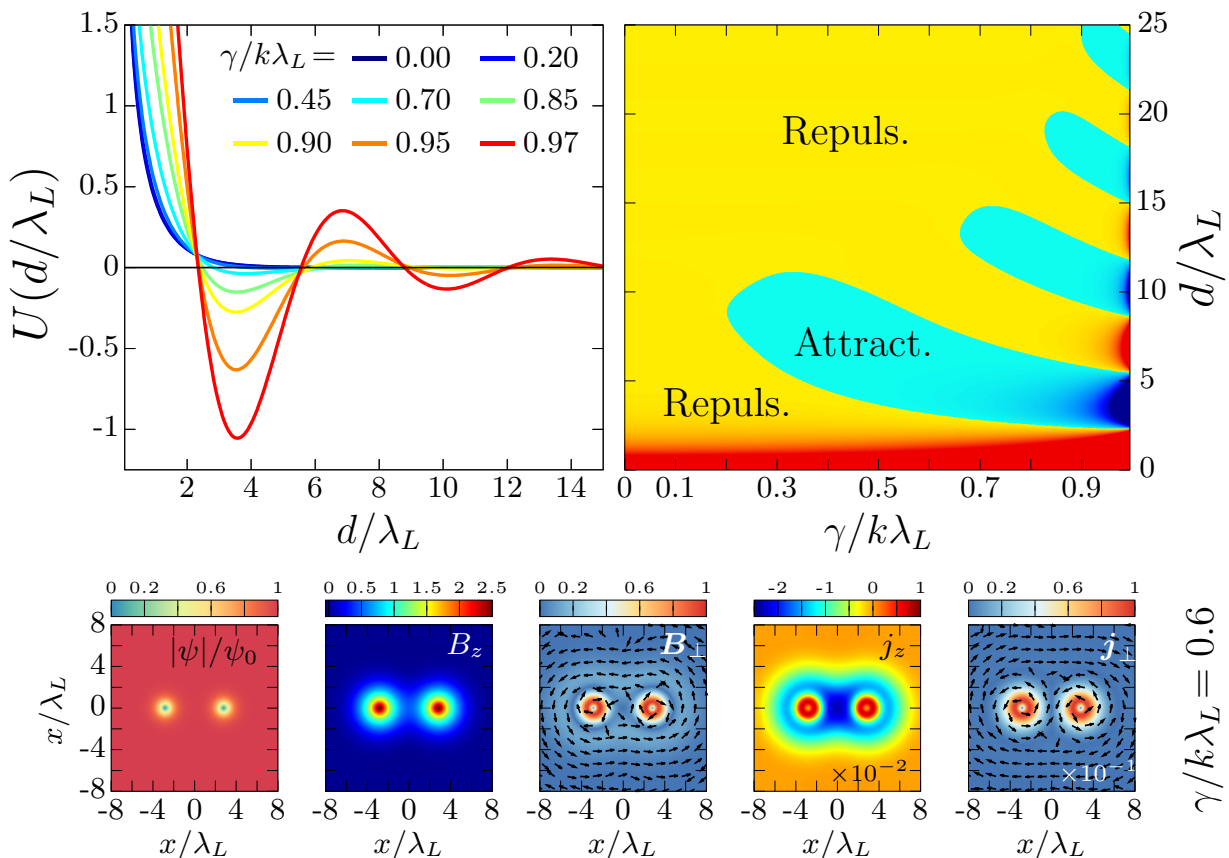


Figure 3. The top-left panel shows the function $U(d/\lambda_L)$ that controls the intervortex interactions, as a function of the distance d between the vortices, for various values of the parity-odd coupling γ . The top-right panel displays a phase diagram showing the attractive and repulsive regions depending on the parity breaking coupling γ and the intervortex distance d . The panels in the bottom row show various physical quantities in the transverse plane of a vortex bound state, for the parity-breaking coupling $\gamma = 0.6\gamma_*$. This vortex pair, obtained after convergence of minimization of the Ginzburg-Landau free energy, demonstrates that the property of the non-monotonic interactions can survive beyond the London limit.

The two dimensional integration in (22) can further be simplified and finally, the free energy reads as:

$$F = \frac{\Phi_0^2(1-\Gamma^2)}{8\pi\lambda_L} \sum_{a,b=1}^N n_a n_b U\left(\frac{|x_a - x_b|}{\lambda_L}\right) \quad (23)$$

$$\text{where } U(x) = \int \frac{q(1+q^2)}{(1+q^2)^2 - 4\Gamma^2 q^2} J_0(qx) dq.$$

Hence the free energy of a set of vortices reads as follows:

$$F = F_0 + \frac{\Phi_0^2(1-\Gamma^2)}{4\pi\lambda_L} \sum_{a,b>a}^N n_a n_b U\left(\frac{|x_a - x_b|}{\lambda_L}\right), \quad (24)$$

where the term $F_0 = \frac{\Phi_0^2(1-\Gamma^2)}{8\pi\lambda_L} \sum_a n_a^2 U(\xi)$ accounts for the self-energy of individual vortices. Since $U(x)$ diverges at small separations x , the self energy has to be regularized at the coherence length $\xi \ll \lambda_L$ which determines the size of the vortex core. The interaction energy of the vortices separated by a distance d is thus determined by the function $U(d/\lambda_L)$. In the absence of parity-breaking

($\Gamma = 0$), the integral in (23) can be calculated analytically, providing again the textbook expression, for the interaction energy $V_{\text{int}}(d/\lambda_L) = \Phi_0^2 K_0(d/\lambda_L)/4\pi\lambda_L$.

Figure 3 displays the function $U(d/\lambda_L)$ which controls the interacting potential between vortices, calculated in the London limit. For vanishing γ , the interaction is purely repulsive, and it is altered by a nonzero coupling. As shown on the left panel, when increasing $\gamma/k\lambda_L$ the interaction can become non-monotonic with a minimum at a finite distance of about $4\lambda_L$. Upon further increase of the coupling γ toward the critical coupling γ_* , the interacting potential can even develop several local minima. The phase diagram on the right panel of Fig. 3 shows the different attractive and repulsive regions as functions of γ and of the vortex separation.

The fact that the interaction energy features a minimum at a finite distance implies that a pair of vortices tends to form a bound state. As can be seen in the bottom row of Fig. 3, the tendency of vortices to form bound states persists beyond the London limit approximation. This configuration is obtained numerically by minimizing the Ginzburg-Landau free energy (1). Notice that

these bottom panels show close-up view of the vortex pair, while the actual numerical domain is much larger [24]. The fact that vortices can form a bound state can heuristically be understood as a compromise between the axial magnetic repulsion of B_z which competes with in-plane attraction mediated by B_\perp . The bound state formation can alternatively be understood to originate from the competition between the in-plane and axial contributions of the currents. First of all, the in-plane screening currents mediate, as usual, repulsion between vortices. The interaction between axial component of the currents, on the other hand, mediates an attraction, just like the force between parallel wires carrying co-directed currents.

The non-monotonic behavior of the magnetic field and currents thus leads to non-monotonic intervortex interactions, and therefore allows for bound state of vortices or cluster to form. Such a situation is known to exist in multicomponent superconductors due to the competition between various length scales (see e.g. [25–29]). In an applied external field, the existence of non-monotonic interactions allows for a macroscopic phase separation into domains of vortex clusters and vortex-less Meissner domains. The situation here contrasts with the multicomponent case, as it occurs only due to the existence of Lifshitz invariants. In two-dimensional systems of interacting particles, multi-scale potentials and non-monotonic interactions are known to be responsible for the formation of rich hierarchical structures. These structures include clusters of clusters, concentric rings, clusters inside a ring, or stripes [30, 31]. It thus can be expected that very rich structures would appear in non-centrosymmetric superconductors as well. However, a verification of this conjecture is beyond the scope of the current work, as it deserves a separate detailed investigation.

As shown in Fig. 3, the interaction energy $V_{v/v}(x) \propto U(x)$ between two vortices with unit winding $n_1 = n_2 = 1$ can thus lead to the formation of a vortex bound state. A very interesting property is that it also opens the possibility of vortex/anti-vortex bound states. Indeed, according to Eq. (24) the interaction of a vortex $n_1 = 1$ and an anti-vortex $n_2 = -1$ corresponds to a reversal of the interacting potential: $V_{v/av}(x) \propto -U(x)$. Thus from Fig. 3 it is clear that if a vortex/anti-vortex pair is small enough, it will collapse to zero size and thus lead to the vortex/anti-vortex annihilation. Now, if the size of the vortex/anti-vortex pair is larger than $4\lambda_L$, there exists an energy barrier that prevents the pair from further collapse. Hence the vortex/anti-vortex pair should relax to a local minimum of the interaction energy. The resulting vortex/anti-vortex bound state has thus a size of approximately $7\lambda_L$.

We find that the most interesting physical effects appear when the parity-breaking coupling γ of the Lifshitz invariant becomes non-negligible with respect to the critical coupling γ_* . The actual values of the coefficients in front of the Lifshitz invariant in the Ginzburg-Landau theory are hard to specify. Unfortunately, for

all presently known non-centrosymmetric materials with O point group symmetry, weak coupling estimates suggest that the parity-breaking coupling is small $\gamma \ll \gamma_*$. However, there are a priori no known theoretical restrictions on the existence of superconducting systems with a strong breaking of the inversion parity. If such materials exist, then according to our analysis they should exhibit the exotic vortex properties investigated here.

V. CONCLUSIONS

In this paper we have demonstrated that the vortices in non-centrosymmetric cubic superconductors feature unusual properties induced by the possible reversal of the magnetic field around them. Indeed, the longitudinal (i.e., parallel to the vortex line) component of the magnetic field changes sign at a certain distance away from the vortex core. Contrary to the vortices in a conventional superconductor, the magnetic-field reversal in the parity-broken superconductor leads to non-monotonic intervortex forces which can act both attractively and repulsively depending on the distance separating individual vortices.

We have demonstrated these properties using mostly analytical calculations in the London limit. Full nonlinear numerical analysis within the Ginzburg-Landau description proves that these properties of non-centrosymmetric superconductors survive beyond the London approximation.

Due to the nonmonotonic intervortex interactions, the vortices in the parity-breaking superconductors may form unusual states of vortex matter, such as bound states and clusters of vortices. The structure of the interaction potential strongly suggests that very rich vortex matter structures can emerge. For example, hierarchically structured quasi-regular vortex clusters, stripes and more, are typical features of the interacting multi-scale and non-monotonic interaction potentials [30, 31].

Moreover, given the possibility to form vortex/anti-vortex bound states, we can anticipate important consequences for the statistical properties and phase transitions in such models.

Note added: In the process of completion of this work, we were informed about an independent work by Samoilenka and Babaev [32] showing similar results about vortices and their interactions. The submission of this work was coordinated with that of [32].

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Appendix A: Positive definiteness of the energy

The free energy (1) should be bounded from below in order to be able to describe the ground state of the NCS superconductor. To demonstrate the boundedness, we use the relations

$$\mathbf{j} = 2e|\psi|^2 (\nabla\varphi - e\mathbf{A}), \quad (\text{A1a})$$

$$|\mathbf{D}\psi|^2 = (\nabla|\psi|)^2 + |\psi|^2 (\nabla\varphi - e\mathbf{A})^2 \quad (\text{A1b})$$

$$= (\nabla|\psi|)^2 + \frac{|\mathbf{j}|^2}{4e^2|\psi|^2}, \quad (\text{A1c})$$

to rewrite the energy density in the following form:

$$\mathcal{F} = \frac{\mathbf{B}^2}{8\pi} + k(\nabla|\psi|)^2 + \frac{k|\mathbf{j}|^2}{4e^2|\psi|^2} + \gamma\mathbf{j} \cdot \mathbf{B} + V[\psi] \quad (\text{A2a})$$

$$= \frac{1}{8\pi} [\mathbf{B}^2 + 8\pi\gamma\mathbf{j} \cdot \mathbf{B}] + \frac{k|\mathbf{j}|^2}{4e^2|\psi|^2} + k(\nabla|\psi|)^2 + \frac{\beta}{2}(|\psi|^2 - \psi_0^2)^2 \quad (\text{A2b})$$

$$= \frac{1}{8\pi} |\mathbf{B} + 4\pi\gamma\mathbf{j}|^2 + \left(\frac{k}{4e^2|\psi|^2} - 2\pi\gamma^2 \right) |\mathbf{j}|^2 + k(\nabla|\psi|)^2 + \frac{\beta}{2}(|\psi|^2 - \psi_0^2)^2. \quad (\text{A2c})$$

Leaving aside all terms with the perfect squares in Eq. (A2c), we find that the only criterion for the free energy to be bounded from below is to require the prefactor in front of the $|\mathbf{j}|^2$ term to be positive. We arrive to the following condition of the stability of the system (1):

$$\gamma^2 < \frac{k}{8\pi e^2 |\psi|^2}. \quad (\text{A3})$$

In the ground state with $|\psi| = \psi_0$, the stability condition (A3) reduces to the simple inequality:

$$\gamma < \gamma_* = k\lambda_L. \quad (\text{A4})$$

where λ_L is the London penetration depth (4).

In the London limit, the superconducting density $|\psi|^2$ is a fixed constant quantity regardless of the external conditions. Therefore the Ginzburg-Landau theory for the NCS superconductor in the London limit is always bounded from below provided the Lifshitz-invariant coupling γ satisfies Eq. (A4).

Positive definiteness beyond London limit

The issue of the positive definiteness is less obvious beyond the London limit. Indeed, let us first assume that the values of the parameters (e, k, γ) are chosen in such a way the formal criterium (A3) is satisfied. If we neglect the fluctuations of the condensate ψ (this requirement is always satisfied in the London regime) then we indeed find that the ground state resides in a locally stable regime so that all terms in the free energy (A2c) are positive defined. However, the density $|\psi|$ is, in principle, allowed to take any value and large enough fluctuations of $|\psi|$ might trigger an instability. A possible signature of the instability can indeed be spotted in the property that a variation of the absolute value of the condensate about the ground state, $|\psi| = \psi_0 + \delta|\psi|$ gives a negative contribution to the free energy, $\delta F = -k\delta|\psi|/(2e^2\psi_0^3)$ in the linear order, provided all other parameters are fixed.

In order to illustrate a possible mechanism of the development of the instability inside the non-centrosymmetric superconductor, let us consider a large enough local region characterized by a uniform, coordinate-independent condensate ψ . For this configuration, the third (gradient) term in the free energy density (A2c) is identically zero. Gradually increasing the value of the condensate beyond the ground state value ψ_0 , we increase the fourth (potential) term in Eq. (A2c) which make this change energetically unfavorable. On the other hand, as the condensate crosses the threshold of the applicability of Eq. (A3), then the second term in the free energy (A2c) becomes negatively defined, and the development of the current \mathbf{j} leads to the unbounded decrease this term. The rise of in the current \mathbf{j} will, in turn, affect the first (magnetic) term, what may be compensated by a rearranging of the magnetic field \mathbf{B} with the local environment in such a way that the combination $\mathbf{B} + 4\pi\gamma\mathbf{j}$ keeps a small value in the discussed region.

Notice that the presence of isolated vortices make the system stable as in a vortex core the condensate vanishes, $\psi \rightarrow 0$, and the second, potentially-unbounded term in (A2c) becomes positively defined. In our numerical simulations we were also spotting certain unstable patterns especially in the regimes when the Lifshitz-invariant coupling γ was chosen to close to the critical value γ_* in the ground state (A4). For example, a system of randomly placed multiple elementary vortices relax their free energy via mutual attraction and formation of a common bound state. Since the vortex bound state hosts a stronger circular electric current, it becomes possible to

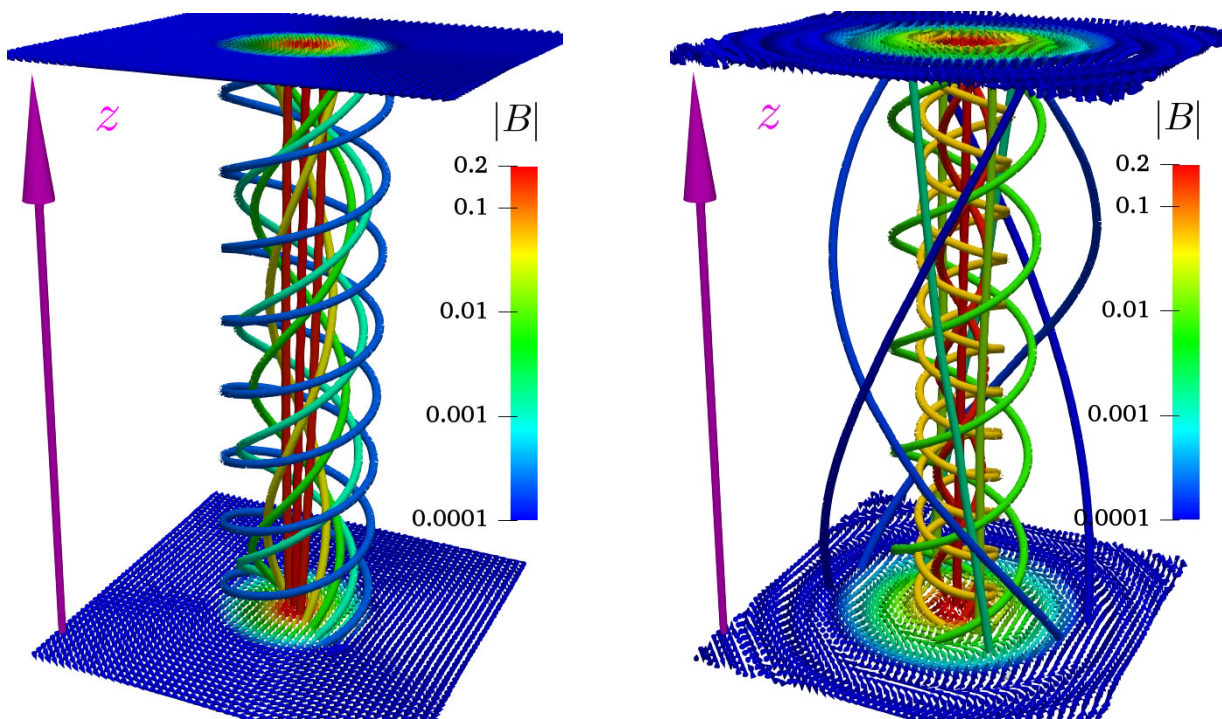


Figure 4. Helical structure of the magnetic field streamlines around vortices in non-centrosymmetric superconductors. The magnetic field is displayed on the two planes normal with respect to the vortex line. The colors encode the amplitude $|B|$, while the arrows demonstrate the orientation of the field. The tubes represent streamlines of the magnetic magnetic field between both planes. The left panel shows the helical structure of the streamlines for moderate value of the parity-breaking coupling $\gamma/k\lambda = 0.2$. The streamlines here feature all the same chirality. The right panel corresponds to rather important parity-breaking coupling $\gamma/k\lambda = 0.8$, for which the longitudinal component of the magnetic field is inverted at some distance from the core. The chirality of the streamline depends on whether the longitudinal component of the magnetic field is inverted.

overcome the stability by ‘compressing’ the vortex cluster, and then destabilizing the whole system.

We conclude that the processes that permit fluctuations of the condensate $|\psi|$ towards the large values (as compared to the ground state value ψ_0) could activate the destabilization of the whole model. Theoretically, the unboundedness of the free energy from below may appear to be an unwanted feature of the model. However, one should always keep in mind that the Ginzburg-Landau functional is a leading part of the gradient expansion of an effective model, and there always exist higher power gradients that will play a stabilizing role preventing the unboundedness to be actually realized in a physically relevant model.

Appendix B: Vortex helicity

As emphasized in the main body of the paper, the magnetic field of vortex states in cubic non-centrosymmetric superconductors feature helicoidal structure around the core. This is illustrated in Fig. 4, that displays typical magnetic field structure around vortex cores. Fig. 4 shows two qualitatively different situation of moderate (left panel) and important (right panel) parity-breaking coupling γ . For moderate parity-breaking coupling, the magnetic field streamlines have helical structure with a pitch that varies with the distance from the vortex core. Note that all streamlines have the same chirality, which is specified by the sign of the parity-breaking coupling γ . On the other hand, as discussed in the main body, vortices features inversion of the magnetic field \mathbf{B} for important parity-breaking coupling γ . As a result, the chirality of the streamline depends on whether the longitudinal component of the magnetic field is inverted. More details about the helical structure of the magnetic field can be seen from animations in Supplemental material [19].