Nematic Skyrmions in Odd-Parity Superconductors

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We study topological excitations in two-component nematic superconductors, with a particular focus on $Cu_xBi₂Se₃$ as a candidate material. We find that the lowest-energy topological excitations are coreless vortices: a bound state of two spatially separated half-quantum vortices. These objects are nematic Skyrmions, since they are characterized by an additional topological charge. The inter-Skyrmion forces are dipolar in this model, i.e., attractive for certain relative orientations of the Skyrmions, hence forming multi-Skyrmion bound states.

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Bulk superconductivity in topological insulator materials has recently been observed in electron-doped $Cu_xBi_2Se_3$ in Refs. [\[1](#page-4-0)–3], and unusual superconducting states in this system were theoretically considered in Ref. [\[4\]](#page-4-1). There, it was argued that the fully gapped single-order parameter superconductor, which has a spin-triplet pairing with odd parity and that possesses topologically protected gapless surface states, is favored over other superconducting states. It was later put forward [\[5\]](#page-4-2) that the interplay of the crystal lattice anisotropy and the nematic superconductivity might be consistent with Knight-shift anisotropy measurements in $Cu_xBi₂Se₃$ that show spontaneous breaking of the spinrotation symmetry below the superconducting transition temperature [\[6\]](#page-4-3). In this model, the nematic superconducting state has an odd-parity spin-triplet pairing and is described by a two-component order parameter that spontaneously breaks the rotational symmetry in the basal plane of the lattice. This scenario of nematic superconductivity is supported by the recent observation of twofold rotational symmetry of the magnetic field in specific heat and upper critical field measurements of the superconducting state [\[7\]](#page-4-4). Bulk superconductivity was also reported in $Sr_xBi₂Se₃$ $[8-10]$ $[8-10]$ and in magnetically doped $Nb_xBi₂Se₃$ [\[11,12\]](#page-4-6), where upper critical field [\[10\]](#page-4-7) and magnetic torque mea-surements [\[12\]](#page-4-8) reveal signatures of rotational symmetry breaking in the amplitude of the superconducting gap.

Nematic superconducting states have interesting properties that were recently theoretically addressed. For example, such states show a specific anisotropy of the upper critical magnetic field [\[13\],](#page-4-9) undergo phase transitions to superconducting states that break the time-reversal symmetry as a result of the interplay of ferromagnetism and superconductivity [\[14,15\],](#page-4-10) and host Majorana fermions at the surface [\[16,17\].](#page-4-11) This raises the question of the properties of topological excitations in this kind of materials. Recent work [\[18\]](#page-4-12) presented an ansatz-based investigation of Kramers pairs of Majorana fermions bound inside a specific type of composite vortices that do not carry

magnetic flux. In the model that we consider below, such an ansatz describes unstable vortex solutions.

In this Letter, we address the question of the nature of the lowest-energy vortex excitations in nematic superconductors. To this end, we investigate vortex solutions in a twocomponent Ginzburg-Landau (GL) model consistently derived from the microscopic theory. We find that the lowest-energy topological excitations are coreless and consist of two spatially separated half-quantum vortices (HQVs) [\[19\],](#page-4-13) such that the total superconducting density has no zeros. These excitations can be characterized by a Skyrmion topological index, which is zero for singular vortices. Heuristically, the Skyrmion terminology follows from the fact that the coreless vortex can be seen as a texture of a unit vector that fully covers the target two-sphere. The unit vector that maps to the target two-sphere is defined as a projection of the superconducting degrees of freedom (d.o.f.) onto the vector composed of the Pauli matrix set.

Such a coreless vortex, which is a bound state of two HQVs, shows as a dipolelike configuration of the relative phase between the components of the order parameter and thus can mediate a long-range dipole interaction between the Skyrmions, thus binding them together into a multi-Skyrmion bound state.

We consider a model of a three-dimensional topological insulator in the presence of a magnetic field, having in mind $Bi₂Se₃$ as a particular material candidate, which is a narrow gap semiconductor with a layered crystal structure. The system is described by the Hamiltonian $\mathcal{H} =$ $\int \Psi^{\dagger}(\mathbf{r})H(\mathbf{r})\Psi(\mathbf{r})d^3r$, with

$$
H(\mathbf{r}) = v\tau_z \left[\boldsymbol{\sigma} \times \left(-i \boldsymbol{\nabla} - \frac{e}{c} \mathbf{A}(\mathbf{r}) \right) \right] \cdot \hat{z} + v_z \tau_y \left(-i \boldsymbol{\nabla}_z - \frac{e}{c} A_z(\mathbf{r}) \right) + m \tau_x, \qquad (1)
$$

where $A(r)$ is the vector potential, $e < 0$ is the electric charge, and m describes the coupling between the orbitals of $Bi₂Se₃$. Here, v and v_z are the Fermi velocities that characterize the anisotropic dispersion of the massive Dirac fermion in the absence of the magnetic field: $E_{\pm}(\mathbf{p}) = \pm \{v^2(p_x^2 + p_y^2) + v_z^2 p_z^2 + m^2\}^{1/2}$, where $\mathbf{p} =$
(p, p, p) is the momentum of a particle. The Pauli (p_x, p_y, p_z) is the momentum of a particle. The Pauli
matrices σ and σ (with $q = x, y, z$) respectively describe matrices σ_a and τ_a (with $a = x, y, z$), respectively, describe the real spin (\uparrow , \downarrow) and the orbital pseudospin (1,2) d.o.f. The electron operator is given by $\Psi(\mathbf{r}) = (\Psi_{\uparrow,1}(\mathbf{r}), \Psi_{\downarrow,1}(\mathbf{r}))$ $\Psi_{\uparrow,2}(\mathbf{r}), \Psi_{\downarrow,2}(\mathbf{r}))^T$, $\hbar = 1$ units are used here, and spin and pseudospin indices are omitted for clarity of notation throughout the Letter. The Zeeman contribution of the magnetic field to the Hamiltonian [\(1\)](#page-0-0) is neglected compared to that of the orbital effect. We also note that, although there is strong spin-orbit interaction in each orbital, the inversion symmetry of the system is preserved.

As demonstrated in Ref. [\[4\]](#page-4-1), the electron-phonon interaction might lead to several distinct s-wave superconducting instabilities in this system: intraorbital spin singlet, interorbital spin singlet, and interorbital spin triplet. Motivated by the experimental signatures for nematic superconductivity, we focus here on the interorbital spin-triplet pairing, which is described by the interaction Hamiltonian within the Bardeen-Cooper-Schrieffer (BCS) approximation:

$$
\mathcal{H}_{\rm BCS} = -\sum_{\sigma,\sigma'} \int d^3r [\Psi^{\dagger}_{\sigma 1}(\mathbf{r}) \Psi^{\dagger}_{\sigma' 2}(\mathbf{r}) \Delta_{\sigma'\sigma}(\mathbf{r}) + \text{H.c.}], \quad (2)
$$

where $\Delta_{\sigma'\sigma}(\mathbf{r}) = \lambda \langle \Psi_{\sigma'2}(\mathbf{r}) \Psi_{\sigma1}(\mathbf{r}) \rangle$ with the interaction constant $\lambda > 0$. Note that we consider the zero harmonic of the stant $\lambda > 0$. Note that we consider the zero harmonic of the electron-phonon interaction potential, which shall give a higher temperature of the superconductor-metal phase transition than higher harmonics. To proceed, we introduce the Bogoliubov–de Gennes (BdG) Hamiltonian \mathcal{H}_{BdG} = $\frac{1}{2} \int \Phi^{\dagger}(\mathbf{r}) H_{BdG}(\mathbf{r}) \Phi(\mathbf{r}) d^3 r$, where

$$
H_{\text{BdG}}(\mathbf{r}) = \begin{bmatrix} H(\mathbf{r}) - \mu & \Delta(\mathbf{r}) \\ \Delta^+(\mathbf{r}) & -\sigma_y H^*(\mathbf{r})\sigma_y + \mu \end{bmatrix}
$$
 (3)

is written in the Nambu notation: $\Phi^{\dagger}(\mathbf{r}) = (\Psi^{\dagger}(\mathbf{r}),$ $\Psi^{T}(\mathbf{r})(-i\sigma_{v})$. We assume the Fermi level to be in the conduction band and hence set $\mu > |m|$. In what follows, we consider the interorbital spin-triplet pairing of the form $\Delta(\mathbf{r}) = \boldsymbol{\sigma} \cdot \boldsymbol{\Delta}(\mathbf{r}) \tau_{v}$, where $\Delta(\mathbf{r}) = [\Delta_{x}(\mathbf{r}), \Delta_{v}(\mathbf{r}), 0]$, such that $\Delta_{\chi}(\mathbf{r}) = -i[\Delta_{\uparrow\uparrow}(\mathbf{r}) - \Delta_{\downarrow\downarrow}(\mathbf{r})]/2$, and $\Delta_{\gamma}(\mathbf{r}) = -[\Delta_{\uparrow\uparrow}(\mathbf{r}) +$ $\Delta_{\perp}(\mathbf{r})/2$. The strong spin-orbit interaction locks electron spin to the momentum, thus fixing the orientation of vector Δ to $[\Delta_x(\mathbf{r}), \Delta_y(\mathbf{r}), 0].$

In order to investigate the structure of the topological excitations, we derive microscopically the GL free energy functional for the two-component order parameter $\Delta_{\pm} = (\Delta_x \pm i\Delta_y)/\sqrt{2}$ (for details of the derivation see Supplemental Material [221]. The scaled derivation, see Supplemental Material [\[22\]\)](#page-4-14). The scaled Ginzburg-Landau free energy functional reads as $4\pi F =$ $h_0^2 l_m^3 \int {\{\mathcal{F}(\mathbf{R}) + [\nabla \times \mathbf{a}(\mathbf{R})]^2\} d^3R}$, where

$$
\mathcal{F} = \sum_{s=\pm} \left(-|\Delta_s|^2 + |D_x \Delta_s|^2 + |D_y \Delta_s|^2 + \beta_z |D_z \Delta_s|^2 + \beta_\perp (D_{-s} \Delta_s)^* D_s \Delta_{-s} + \frac{|\Delta_s|^4}{2} + \frac{\gamma}{2} |\Delta_s|^2 |\Delta_{-s}|^2 \right), \quad (4)
$$

where $\Delta_{\pm} = |\Delta_{\pm}|e^{i\varphi_{\pm}}$. Here we have defined the order
parameter Δ (**R**) in the scaled form. The explicit scaling parameter $\Delta_{s}(\mathbf{R})$ in the scaled form. The explicit scaling transformation for coordinate **R**, vector potential $\mathbf{a}(\mathbf{R})$, and operator $D_{\pm} = D_x \pm iD_y$ in which $\mathbf{D} = -(i/\kappa)\nabla_R + \mathbf{a}(\mathbf{R})$
is given in Supplemental material [22]. In dimensionless is given in Supplemental material [\[22\].](#page-4-14) In dimensionless units, the coupling constant κ parametrizes the magnetic field penetration length relative to a characteristic length scale associated with density variation. Its explicit expression through the parameters of the microscopic model is given in Supplemental Material [\[22\]](#page-4-14) [Eq. (F.73)], as well as the expression for other coefficients h_0 , l_m , β_{\perp} , and γ . For $\kappa \ll 1$, the vortex core energy is relatively large and the thermodynamically stable Skyrmions do not form.

The anisotropy of the electronic spectrum results in the anisotropic gradient terms on the first line of the GL functional [\(4\).](#page-1-0) The interplay of the two-component order parameter and strong spin-orbit interaction gives rise to the mixed gradient term with the coefficient $0 < \beta_{\perp} < 1$ on the second line in Eq. [\(4\).](#page-1-0) The GL free energy functional density is invariant under the joint rotation of coordinates and the components of the order parameter [\[23\]](#page-4-15). Finally, the value of γ determines whether the superconductor is in the nematic $0 < \gamma < 1$ or in the chiral $\gamma > 1$ phase. Indeed, in the spatially homogeneous case, when $0 < \gamma < 1$ the free energy is minimal if the order parameter has the form $\Delta = \Delta_0(\cos \theta, \sin \theta, 0)$ (for some real constant θ and $|\Delta_0| = 1/\sqrt{1+\gamma}$, while it reads as $\Delta = \tilde{\Delta}_0(1, \pm i, 0)$
(where $|\tilde{\Delta}| = 1$) when $\mu > 1$ (where $|\Delta_0| = 1$) when $\gamma > 1$.

Time-reversal symmetry is preserved in the nematic state. The chiral state, on the other hand, is characterized by the nonzero electron spin polarization $\alpha |\Delta(\mathbf{r}) \times \Delta^*(\mathbf{r})| \neq 0$. Interestingly, nontrivial pseudospin polarization, antiferromagnetic spin orientation in two orbitals, shows up in the first gradients of the order parameter in both the chiral and nematic cases; see Supplemental Material [\[22\].](#page-4-14)

The GL equation for the component Δ_s of the order parameter is obtained by the functional variation of Eq. [\(4\)](#page-1-0) with respect to Δ_s^* :

$$
(D_x^2 + D_y^2 + \beta_z D_z^2)\Delta_s + (|\Delta_s|^2 + \gamma |\Delta_{-s}|^2 - 1)\Delta_s
$$

= $-\beta_\perp D_s^2 \Delta_{-s}$ (5)

and is supplemented by the boundary condition

$$
\mathbf{N} \cdot \mathbf{D} \Delta_s + (\beta_z - 1) N_z D_z \Delta_s + N_s D_s \Delta_{-s}|_{\text{surf}} = 0, \quad (6)
$$

where $N_s = N_x + i s N_y$ and N is the unit vector directed normal to the surface. Note that here we do not consider the effects of the localized surface states. Finally, the vector

$$
-2\mathbf{\nabla} \times \mathbf{b} = \sum_{s=\pm} \{ [\Delta_s^* \mathbf{D} \Delta_s + (\beta_z - 1) \Delta_s^* \hat{z} D_z \Delta_s + \text{c.c.}] + (\hat{x} + i s \hat{y}) \beta_\perp [\Delta_s^* D_s \Delta_{-s} + \Delta_{-s} (D_{-s} \Delta_s)^*] \}.
$$
 (7)

We now turn to the investigation of the nature of topological excitations in the nematic superconductor. In two-component models, due to the coupling of the components to the vector potential $a(R)$, the only solutions with finite energy per unit length have the same phase winding in both components of the order parameter, that is, a bound state of vortices in the different components, each carrying a fraction of magnetic flux that adds up to a single flux quantum. In the current model of the nematic superconductor, vortices in each component of the order parameter carry half of a magnetic flux quantum; hence, they are halfquantum vortices (HQVs) [\[24\]](#page-4-16). Typically, the magnetic interaction between HQVs favors cocentricity of the vortex cores in the different components (see, e.g., a detailed discussion in Ref. [\[25\]](#page-4-17)). On the other hand, the model considered here also features mixed gradients and biquadratic density-density terms that result in the repulsion between the cores of the half-quantum vortices. Provided the latter dominate, the competition between those forces may result in a bound state of nonoverlapping half-quantum vortices, thus breaking the axial symmetry of the solution.

To address whether vortices are singular (cocentered HQV) or coreless (i.e., noncocentered HQV), we numerically construct vortex solutions by minimizing the free energy [\(4\)](#page-1-0), starting by an initial configuration, in which both components Δ_{\pm} have the same winding. The theory is discretized within a finite-element formulation [26] and discretized within a finite-element formulation [\[26\]](#page-5-0) and minimized using a nonlinear conjugate gradient algorithm [\[27\]](#page-5-1). Minimization procedure leads, after the convergence of the algorithm, to a vortex configuration that carries a number of flux quanta that is specified by the initial phase winding. Figure [1](#page-2-0) shows such a single-quantum vortex configuration in the model [\(4\)](#page-1-0) for the nematic superconductor. Note that the picture shows a close-up view, displaying only a small part of the simulated numerical grid, which is chosen to be large enough so that vortices do not interact with the boundaries. Clearly, the vortex solution is not axially symmetric. Inspection of the core structure reveals that HQVs in different components are spatially separated and thus that this bound state of HQVs is coreless; i.e., there is no singularity of total density of superconducting components: $[|\Delta_+(\mathbf{R})|^2 + |\Delta_-(\mathbf{R})|^2]^{1/2}$. We simulated vortex solutions for various initial guesses that always converge to configufor various initial guesses that always converge to configu-rations as in Fig. [1.](#page-2-0) All investigated values of the parameter κ led to coreless vortices in the type-II regime. The distance between HQVs is determined by the competition between magnetic attraction and repulsion mediated by other terms such as density-density interaction. This cannot be

FIG. 1. Close-up view of the vortex core structure in the nematic phase in which we set $v = v_z$, $\beta_z = 0$, and for $\kappa = 3$. On the first line, the first panel shows the distribution of the magnetic field, while the second displays the relative phase between the two components of the order parameter. The second line shows the densities of the two components of the order parameter. Clearly, the cores in both components do not superimpose, thus implying that vortices in the nematic phase are coreless defects. Since cores do not overlap, the relative phase has -exhibits a dipolar mode that is long-ranged. $\pm 2\pi$ winding around each core. Furthermore, the relative phase

addressed analytically, but quantitatively it can be seen that increasing the value of κ decreases binding the HQVs, thus increasing their separation. Since the superconductor is substantially away from the type-I regime, and because these excitations are energetically cheaper than singular vortices, a lattice of Skyrmions will form in the external field.

As singularities in both components do not overlap, there is a dipolelike configuration of the relative phase $\varphi = -\varphi_{+}$ between the components. Importantly, the phase-difference gradients are very strong. This indicates that intervortex forces include torque and a long-range dipole interaction that can lead to a long-range attraction between singlequanta vortices. As displayed in Fig. [2](#page-3-0), by initially setting a double phase winding in each component, we find that indeed two single-quantum vortices form a bound state due to the dipolar forces. Note that the presence of dipolar interactions usually has clear signatures in structure formation. In particular, studies of Skyrmion solutions in other systems with dipolar inter-Skyrmion forces [\[28](#page-5-2)–30] show, for example, that hexagonal symmetry is unfavorable for the Skyrmion lattices. Moreover, the long-range dipolar interaction can also result in long-range attractive interaction between Skyrmions and boundaries of a superconductor, thus suggesting a possible abundance of topological defects near boundaries in a weak applied magnetic field.

Bound states of nonoverlapping HQVs are coreless defects that can be called Skyrmions, and the reason for that terminology is that they exhibit additional topological

FIG. 2. A close-up view of a bound state of two coreless vortices carrying one flux quantum each. Each coreless vortex is a well-localized bound state of two HQVs. The dipolelike forces in the relative phase yields a long-range attraction that binds the single-quantum vortices together. Note that the dipoles are antialigned in the bound state as dictated by relative phase interaction. Displayed quantities are the same as in Fig. [1](#page-2-0).

properties, as compared to singular vortices. These can be seen by introducing the unit vector n, defined as the projection of the superconducting d.o.f. $\eta^{\dagger} = (\Delta_{+}^{*}, \Delta_{-}^{*})$
onto spin-1/2 Pauli matrices $\tilde{\sigma}$ as $\mathbf{n} = n^{\dagger} \tilde{\sigma} n / n^{\dagger} n$. Then projection of the superconducting d.o.f. $\eta^2 = (\Delta_+, \Delta_-)$
onto spin-1/2 Pauli matrices $\tilde{\sigma}$, as $\mathbf{n} = \eta^{\dagger} \tilde{\sigma} \eta / \eta^{\dagger} \eta$. That
is the x and y components of the vector **n** depend on the is, the x and y components of the vector \bf{n} depend on the phase difference, while the z component is determined by the ratio of the moduli of the complex fields. The associated projection is a map from the one-point compactification of the plane (Re²∪{∞} ≃ S²) onto the two-sphere target space spanned by **n**. That is **n** : $S^2 \rightarrow S^2$, which is classified by the homotopy class $\pi_2(S^2) \in \mathbb{Z}$. This defines the integervalued \mathbb{CP}^1 topological invariant, as

$$
\mathcal{Q}(\mathbf{n}) = \frac{1}{4\pi} \int_{\text{Re}^2} \mathbf{n} \cdot \partial_x \mathbf{n} \times \partial_y \mathbf{n} dx dy.
$$
 (8)

If $\eta \neq 0$ everywhere (coreless vortex), Q is an integer number. In a way, Q counts the number of times the texture of n covers the target two-sphere.

Figure [3](#page-3-1) shows the texture of the unit vector n that corresponds to the vortices in the nematic phase. The left panel corresponds to the single-quantum vortex displayed in Fig. [1.](#page-2-0) It illustrates that the unit vector n wraps the target two-sphere (once), thus implying this configuration has unit Skyrmionic charge $Q = 1$. The right panel shows the texture corresponding to the bound state of Fig. [2](#page-3-0) that originates in long-range dipolelike forces. Note that this illustrates the dipole nature of the long-range interaction. Indeed, the pair of Skyrmions alternates the north (red) and south (blue) poles of the target sphere.

It is worth noting that various coreless vortices were also considered to exist in a number of models of multicomponent superconductivity. There are, however, substantial differences in the structure and properties of these solutions, and they should have distinct experimental manifestations. For example, in the framework of various models of p-wave superconductors, it was advocated that multiquanta coreless vortices may be favored over singlequanta singular vortices [\[32](#page-5-3)–34]. The recent numerical studies show that two-quanta Skyrmions in the GL models of a chiral p-wave superconductor are energetically favored, and hence single-quanta Skyrmions do not form in the ground state in an external field [\[27,31,35](#page-5-1)–37]. Different types of chiral Skyrmions were also discussed for $s + is$ superconducting states [\[31,38,39\].](#page-5-4) The structure of chiral Skyrmions is significantly dissimilar compared to the nematic Skyrmions, since the former have fractional vortices and magnetic flux pinned on domain walls between different

FIG. 3. Texture of the unit vector **n** defined as the projection of the superconducting d.o.f. onto the spin-1/2 Pauli matrices. The left panel shows a single-quanta solution corresponding to Fig. [1,](#page-2-0) while the right panel corresponds to the bound state displayed in Fig. [2.](#page-3-0) Inspection of the single-quanta solution show how n wraps the target two-sphere. The north (respectively, south) pole signals zero of Δ_+ (respectively, Δ−) and thus the position of respective HQVs. From this one, can see structural difference of nematic Skyrmions, compared to Skyrmions in chiral superconductors [\[31\]](#page-5-4). Here the solution has clearly the form of weakly interacting well-separated Skyrmions with unit topological charge each. By contrast, in the chiral case the Skyrmionic topological charge tends to be relatively uniformly spread along closed domain walls.

time-reversal symmetry broken states [\[40\]](#page-5-5); thus, they have very different magnetic field configurations.

The object that we find here should be interesting from the viewpoint of electronic states. Indeed, HQVs are known to possess Majorana modes. The spatial separation between two HQVs in the Skyrmion implies that individual HQVs may be rather easily stabilized in a mesoscopic sample.

In conclusion, we discussed the topological excitations in nematic superconductors. We showed that the topological excitations are nematic Skyrmions, each of which can be viewed as a bound state of two spatially separated half-quantum vortices. The nematic Skyrmions have orientation-dependent dipolar attractive forces and form multiquanta bound states, which could be expected to have clear experimental signatures in structure formation. Moreover, being coreless, the Skyrmions are expected to have unusual electronic core-state properties that could allow the identification of Skyrmionic states using scanning tunneling microscopy.

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