Disclination Classes, Fractional Excitations, and the Melting of Quantum Liquid Crystals

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Disclination classes, fractional excitations, and the melting of quantum liquid crystals

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We consider how fractional excitations bound to a dislocation evolve as the dislocation is separated into a pair of disclinations. We show that some dislocation-bound excitations (such as Majorana modes and half-quantum vortices) are possible only if the elementary dislocation consists of two inequivalent disclinations, as is the case for stripes or square lattices but not for triangular lattices. The existence of multiple inequivalent disclination classes governs the two-dimensional melting of quantum liquid crystals (i.e., nematics and hexatics), determining whether superfluidity and orientational order can simultaneously vanish at a continuous transition.

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Spatial order (i.e., crystallinity) can be found intertwined with exotic quantum-mechanical order in various systems: for instance, with unconventional superfluidity, in the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state and related states [1–7]; and with topological electronic structure, in weak and crystalline topological insulators/superconductors [8–14]. In such cases, the defects of the *translational* crystalline order—i.e., *dislocations*—can bind excitations or defects of the intertwined quantum-mechanical order, such as Majorana bound states, helical edge modes, or half-quantum vortices [15, 16]. More generally, such composite defects and their proliferation are a hallmark of deconfined quantum criticality [17]. A common feature of the dislocation-bound states noted above is that they are "Z_2" in character, i.e., two of them combine to give a conventional bound state which is trivial in some sense.

The fact that dislocations can bind such Z_2 states raises a conceptual puzzle because dislocations are themselves composite defects: a dislocation is a bound state of two *disclinations*, which are topological defects of *orientational* order [18–22]. When a dislocation is split into two widely separated disclinations (Fig. 1), there is *prima facie* no straightforward way for the accompanying bound state to divide or stretch between the two disclinations; nor is there an obvious principle for assigning the bound state to either disclination. In this work we immediately present the resolution to this puzzle by explaining why the bound state attaches itself to one of the two disclinations, and then discuss the non-trivial consequences of this concept.

Following Ref. [23], we note that certain lattices (including stripes and square lattices) have topologically inequivalent classes of *disclinations*, some of which support exotic bound states on their own. We find that a dislocation carrying a Z_2 bound state is *always* composed of one trivial and one nontrivial disclination; when the dislocation splits, the bound state attaches itself to the non-trivial disclination. An immediate corollary is that in lattices without multiple, inequivalent types of disclinations, there will be no non-trivial Z_2 bound states on dislocations either. Using these ideas we show that when translational order is intertwined with superfluidity, the presence, or absence, of multiple disclination classes modifies the structure of the phase diagram in two dimensions. For example, in lattices that have only one class of elementary disclination (e.g., hexagonal lattices [24]), superfluid and liquid-crystalline order can generically vanish at once through a continuous transition; in lattices with inequivalent disclinations, however, this is forbidden except possibly at a multicritical point. While this work only explicitly considers superfluid order, the arguments and main result will also apply to cases where dislocations carry other, perhaps magnetic, defects (as in Refs. [25, 26]).

Our predictions are straightforward to test in ultracold atomic experiments with FFLO liquid crystals or

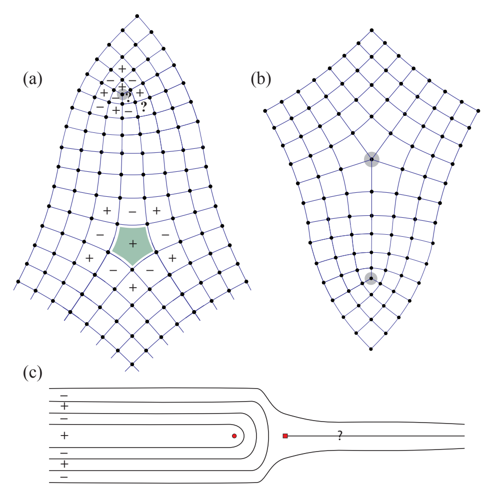

FIG. 1: (a), (b) $\pm\pi/2$-disclination dipoles that fuse into dislocations with odd, even Burgers' vectors respectively. (c) Two inequivalent classes of disclinations of a two-dimensional striped superfluid. Lines denote nodes of the order parameter; the sign of the condensate between these is indicated on the left. The crest-centered disclination (red circle) involves no sign-frustration, whereas the trough-centered disclination (red square) does involve sign-frustration.

spin-orbit coupled condensates [27–33]. Furthermore, our central result regarding inequivalent disclinations has immediate experimental consequences for weak topological insulators and superconductors where our arguments imply that it is the disclination core-size, rather than the dislocation core-size, that sets the scale and spacing of bound states. This prediction is particularly salient to experiments, as the conditions under which dislocations are common and easy to probe (i.e., when crystalline order is weak) are precisely those under which the dislocations consist of two weakly bound disclinations.

Classification of disclinations. We begin by discussing the main result of Ref. [23] on the holonomy-based classification of disclinations. The formal argument is summarized in the Supplemental Material; here, we state the result and provide an intuitive justification. The result can be stated as follows: *a disclination is characterized by (a) an angle θ (the Frank angle), through which the lattice rotates; and (b) a center around which the rotation takes place.* Allowed values for both θ and the center can be determined by looking at global transformations that leave the lattice invariant (i.e., that map the lattice onto itself). Thus, the allowed values of θ are $m\pi/(2n)$, where the lattice is n-fold symmetric; we shall only be concerned with the elementary, π/n disclinations—e.g., the π disclination for a stripe [Fig. 1(c)], the $\pi/2$ disclination for a square lattice [Fig. 1(a)], etc. Now, an allowed θ does *not*, on its own, automatically guarantee invariance. One can see this by trying (for instance) to rotate a stripe by 180 degrees about an arbitrary point: in general, this transformation would lead to a *translated* stripe, and is thus not a symmetry. There are only two centers around which a global π rotation brings a stripe back to itself: these are a *crest* (a point of maximum density) and a *trough* (a point halfway between two crests). Similarly, there are only two centers around which a $\pi/2$ rotation brings a square lattice back to itself: these are a *vertex* or a *plaquette*. For a triangular lattice, one can see that the *only* allowed center for a $\pi/3$ rotation is a vertex.

The result of Ref. [23] is that disclinations with different centers are *inequivalent*, and cannot continuously be transformed into one another. This is easy to see in many concrete examples: for instance, on the square lattice [Fig. 1(a)], the vertex-centered disclination involves one site with an odd coordination number, whereas the plaquette-centered disclination does not. In general, elementary disclinations come in two inequivalent varieties for a stripe (crest- or trough-centered) or a square lattice (vertex- or plaquette-centered), but only one variety for a triangular lattice (vertex-centered). Our central result in what follows is that this classification of disclinations based on inequivalent centers can have a major impact on melting transitions.

Striped superfluids. We now address the nature of disclination-vortex bound states, beginning with the case of a striped superfluid described by a Bose condensate of the form $\psi(\mathbf{x}) = \psi\cos(\mathbf{k}\cdot\mathbf{x}+\phi)\exp(i\theta)$, where ψ is a (fixed) amplitude and θ and ϕ are phases associated with the superfluid and translational Goldstone modes respectively. Examples of such states are the Fulde-Ferrell-Larkin-Ovchinnikov state proposed for spin-polarized superconductors [1–4, 34, 35], and states of ultracold atoms with spin-orbit coupling [29–31, 33, 36]. For specificity, we address the rotationally invariant case; thus, our analysis directly applies to FFLO states and to Bose gases subject to a Rashba spin-orbit coupling [28–30, 33]. However, we could restore weak anisotropy without affecting our conclusions, as discussed below.

The striped superfluid has three easily identifiable topological defects [5]: (i) a pure dislocation, in which ϕ winds by 2π, (ii) a pure vortex, in which θ winds by 2π, and (iii) a half-vortex-dislocation bound state, in which both ϕ and θ wind by π. Since defects (i) and (ii) can be written as dipoles of (iii), it suffices to understand how the vortex-dislocation bound state separates into disclinations. For the striped superfluid there are two types of disclinations, a node-centered one and an antinode-centered one; these two types are affected in very different ways by the sign-changing order parameter. In particular, the sign of the order parameter is *frustrated* around a node-centered disclination, whereas it is not frustrated around an antinode-centered disclination [Fig. 1(c)]. This sign-frustration around a node-centered disclination can precisely be compensated by introducing a half-vortex. Thus, the Z_2 classification of disclinations for stripes provides a direct (and hitherto undiscussed) geometric criterion for understanding how a half-vortex half-dislocation splits. Of the two kinds of possible disclinations, only the node-centered (type-A) disclination binds a vortex, to compensate for the sign-frustration. Therefore, as an elementary vortex-dislocation bound state contains one node-centered and one anti-node centered (type B) disclination, the type-A disclination inherits the half-vortex when the dislocation unbinds.

We turn to the melting of a striped superfluid. In a rotation-invariant two-dimensional system, dislocations proliferate at any nonzero temperature, reducing the smectic to a nematic [3]. In what follows, we consider this nematic; we denote the elementary disclinations and their composites using the notation (α, β) where α is the orientational charge and β is the superfluid charge. A type-A disclination $(1, 1)$ has both superfluid and orientational charge, whereas a type-B disclination $(1, 0)$ has only orientational charge. Thus, a pure dislocation is $(0, 0)$ (and can be constructed as a dipole of two type-A or type-B disclinations with opposite α); a pure vortex has charge $(0, 2)$ and can be composed of two type-A disclinations of opposite α (Frank angle); and finally, a half-vortex half-dislocation bound state consists of one type-A and one type-B disclination, and thus carries charges $(0, 1)$.

The low-energy theory of a nematic superfluid is given, in the one-constant approximation [18], by

$$\mathcal{H}_{el.} = \kappa\left[(\nabla\cdot\mathbf{n})^2 + (\nabla\times\mathbf{n})^2\right] + \rho_s|\nabla\theta|^2, \tag{1}$$

where $\mathbf{n}$ is a unit vector normal to the local orientation of the nematic, κ is the Frank constant governing orientational stiffness, and ρ_s is the superfluid stiffness. This equation can be analyzed using the standard Coulomb gas technique [5, 37] for Kosterlitz-Thouless transitions. (This analysis involves transforming Eq. 1 into a theory in terms of topological defects [5, 37], and then computing the scaling dimensions of various defects.) The result of this analysis is the following criterion for the temperature at which a topological defect with charges (α, β) proliferates (or unbinds) [5]:

$$k_B T_{\alpha\beta} = \frac{\pi}{2}[\alpha^2\kappa + \beta^2\rho_s] \tag{2}$$

We now investigate what this criterion implies for the phase diagram of the nematic superfluid.

In the nematic superfluid, all charge is confined, so that the equilibrium state contains neutral dipoles of two type-A or two type-B disclinations. Type-A disclinations are bound by superfluid *and* orientational charge; thus, they are more tightly bound than type-B disclinations, and cannot proliferate before the type-B disclinations. Thus, we find that there is generically no direct transition from the nematic superfluid to an isotropic normal phase, contrary to Ref. [38]. In the Coulomb gas language, one can see this as follows. Depending on ρ_s/κ, the defects with the lowest threshold for unbinding are type-B disclinations $[(1,0)]$ or orientationally neutral half-vortex half-dislocations $[(0,1)]$; other defects are always less relevant. For small ρ_s/κ, the half-vortex half-dislocation proliferates first, leading to a nematic non-superfluid state. For larger superfluid densities, the type-B disclination proliferates first, leading to an isotropic superfluid. The resulting phase diagram is shown in Fig. 2(a): the two transitions meet at a multicritical point, at $\kappa = \rho_s$, which is the only point at which a direct transition out of the nematic superfluid into a normal phase is possible (although nonlinearities might change the phase diagram near this multicritical point). Note that in experiments with spin-orbit coupled Bose gases, one can tune the ratio κ/ρ_s by tuning the spin-dependent scattering lengths [29–33].

We now turn to hexagonal and square-lattice pair-density waves with sign-changing order parameters. These can arise due to nonlinear interactions between stripes, or can be engineered by tuning interactions (e.g., cavity-mediated [39, 40] or fermion-mediated interactions) peaked at certain momenta. A specific pair-density-wave state on a hexagonal lattice was recently discussed [7] with an analysis that ignored the effects of disclinations. However, disclinations play a crucial role in the melting transition and we find, remarkably, that

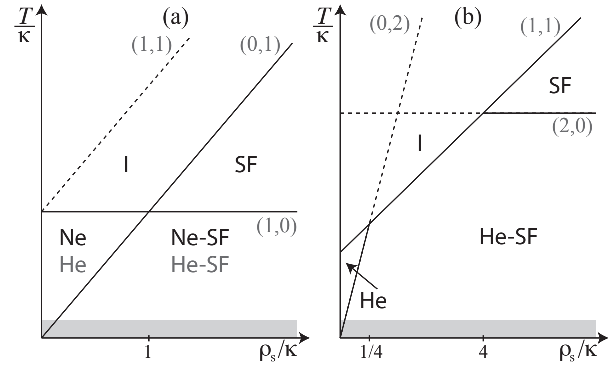

FIG. 2: (a) Phase diagram of a striped, or square-lattice, superfluid in two dimensions, for a fixed Frank constant, as a function of superfluid stiffness and temperature. Solid lines denote phase transitions, due to the proliferation of defects (indexed by their orientational and superfluid charges); the dashed line represents the temperature at which type-A disclinations would (hypothetically) have proliferated if the system were still ordered. The four phases are nematic/hexatic (Ne/He), nematic/hexatic superfluid (Ne/He-SF), isotropic superfluid (SF), and isotropic normal (I). (b) Phase diagram of a triangular-lattice superfluid [case (a)]. The notation is the same as that in (a); note that a direct transition from the hexatic superfluid to the isotropic normal state, absent in (a), appears here.

the nature of two-dimensional melting depends strongly on the lattice geometry, via the classification of disclinations.

Unlike striped states, crystalline states can sustain quasi-long-range order at finite temperatures in two dimensions; however, they generally melt in two steps, with dislocations proliferating first and then disclinations [19–21, 41]. We shall analyze the intermediate "hexatic" phase, in which pure dislocations have proliferated (so that translational order is short-range) but disclinations are confined. For square lattices (i.e., checkerboard arrangements of the order parameter), as with stripes, there are two inequivalent classes of disclinations; only one of the classes has sign-frustration and thus binds a half-vortex [Fig. 1]. Thus, the phase diagram for a square-lattice is exactly as in the striped case: the first defect to proliferate is either the neutral disclination or the vortex-dislocation hybrid, so that the transition out of the hexatic superfluid is into either a hexatic or a superfluid state.

For triangular/hexagonal lattices we must distinguish between two types of configurations: (a) that where the nodes of the order parameter form a triangular lattice [Fig. 3(a)]; and (b) that where the antinodes form a triangular lattice [Fig. 3(b)] and the nodes occupy the dual honeycomb lattice. This complication does not appear in the square lattice because it is self-dual. We consider case (a) first. We see the $\pm\pi/3$ disclinations on the triangular lattice in Fig. 4(e) break the $\bullet, \circ$-sublattice or-

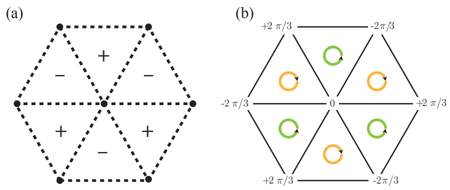

FIG. 3: Two possible varieties of hexagonal-lattice superfluid. (a) Hexagonal lattice of nodes of the order parameter, corresponding to a honeycomb lattice of the particle density, $+,-$ represent the sign of Bose condensate ψ; (b) Hexagonal lattice in the particle density, corresponding to a honeycomb lattice of vortices, $0, \pm 2\pi/3$ are phases of the condensate ψ.

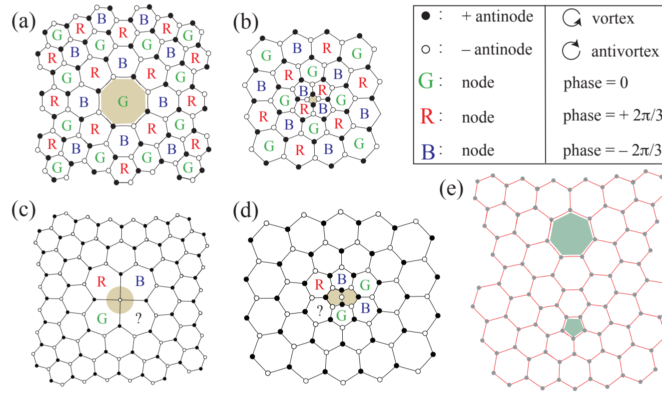

FIG. 4: (a-d) Inequivalent trivial $\pm 2\pi/3$-disclinations. None breaks the $\bullet, \circ$-sublattice order (no nearest vertices are of same type). Tri-coloring ordering (no adjacent plaquettes have same color) is preserved for (a) and (b) and is broken for (c) and (d). (e) Topological $\pm\pi/3$-disclination dipole. Each breaks $\bullet, \circ$-sublattice and tri-coloring order.

der that corresponds to the opposite signs in Fig. 3(a) and therefore invariably carry a half-vortex [i.e. they have charges $(1, 1)$]. These disclinations can be combined to form pure vortices $(0, 2)$ or double disclinations $(2, 0)$ [Fig 4(a-d)]. Depending on ρ_s/κ, any of the three defects might proliferate first. In particular, the proliferation of $(1, 1)$ disclination-vortex states, which is favored when the orientational and superfluid stiffness are comparable [i.e., $1/4 \leq \kappa/\rho_s \leq 4$], can give rise to a direct Kosterlitz-Thouless transition between the nematic superfluid and an isotropic normal state [Fig. 2(b)].

We now briefly comment on case (b), in which the antinodes form a hexagonal lattice [7]; one can alternatively regard this state as a honeycomb lattice in which the $\bullet$-sites are occupied by vortices and the $\circ$-sites by antivortices in Fig 4. Formally, this situation is different from that discussed so far, as the relative phase between neighboring antinodes is not π (i.e., a minus sign) but $2\pi/3$ (graphically, this can be represented as a tri-coloring as in Fig. 4); correspondingly, the fractional vortex [7] has a charge of $1/3$, and is a Z_3 rather than a Z_2 defect. This distinction is crucial, for the following reason: a nontrivial Z_3 defect can bind to a dislocation *even if* the dislocation consists of two equivalent disclinations, because $2 = 1{+}1$ and $1 = 2{+}2 \bmod 3$, so that the original puzzle discussed in the introduction does not apply. For completeness, we show in the Supplemental Material that this case yields a phase diagram of the form in Fig. 2(a); its main significance in the present work, however, is that it provides a simple counterexample, illustrating why the restriction to Z_2 bound states was crucial for our analysis.

Finally, we sketch the implications of our results for weak topological insulators and superconductors. It is known that the presence of low-energy bound states on a dislocation is determined by the weak topological index [15]; as the weak-index is *always* zero for a triangular lattice, it follows that there are no bound states. On the square lattice, one can explicitly see from the construction of Ref. [23] that a weak topological invariant entails inequivalent disclinations. Although no analogous classification of topological insulators (i.e., not assuming particle-hole symmetry) has been performed, one can explicitly see that in the case of a weak topological insulator layered along the z axis, an edge dislocation line along the z axis containing helical edge modes can be decomposed into a disclination line that carries helical modes and one that does not. These observations imply that the transverse size of the bound states is set by that of the *disclination* core, which is typically smaller than the dislocation core. The presence of bound states also generates an effective attraction between disclinations of the same topological type; however, one expects this to fall off exponentially with separation and therefore not to affect melting transitions.

In summary, we have shown that the absence (presence) of inequivalent disclination classes implies that superfluid and liquid-crystalline order can (cannot) be lost at once via a Kosterlitz-Thouless transition. This prediction is straightforward to test experimentally in ultracold atomic gases, as vortex-unbinding can be seen via interferometry [42] and orientational order via time-of-flight imaging [43]. We have argued, further, that the existence of inequivalent disclinations corresponds to a nontrivial weak invariant for topological insulators. The extensions of this classification to states such as nematic Chern insulators [44, 45], and to quantum melting [46, 47] will be considered in future work.

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