Anomalous Coupling Between Topological Defects and Curvature

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We investigate a counterintuitive geometric interaction between defects and curvature in thin layers of superfluids, superconductors, and liquid crystals deposited on curved surfaces. Each defect feels a geometric potential whose functional form is determined only by the shape of the surface, but whose sign and strength depend on the transformation properties of the order parameter. For superfluids and superconductors, the strength of this interaction is proportional to the square of the charge and causes all defects to be repelled (attracted) by regions of positive (negative) Gaussian curvature. For liquid crystals in the one elastic constant approximation, charges between 0 and 4π are attracted by regions of positive curvature while all other charges are repelled.

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The physics of topological defects on curved surfaces plays an increasingly significant role in the engineering of devices based on coated interfaces [1–3]. Defects also affect the mechanical properties of some biological systems, such as spherical viruses, whose shape is dependent on the presence of disclinations in their protein shell [4]. Furthermore, the effects induced by a curved substrate on the distribution of defects are not fully understood even in well studied systems such as thin superfluid or superconducting films. In this Letter, we study simple continuum generalizations of the plane XY model to frozen surfaces of varying curvature to gain a broad understanding of the interaction between topological defects and curvature.

The XY model is a simple setting in which particlelike objects emerge from a more fundamental theory. The basic degree of freedom is an angle-valued function on the plane whose values vary from 0 to 2π. These angles could represent the orientations of interacting arrows. The interaction, which tends to align neighboring arrows, results from the continuum free energy $\mathcal{F}$ given by

$$\mathcal{F} = \frac{K}{2}\int d^2\mathbf{u}[\nabla\theta(\mathbf{u})]^2, \tag{1}$$

where the set of coordinates $\mathbf{u} = (x, y)$ label points on the plane. Despite its simplicity, this model captures the main properties of vortices in layers of superfluid ^{4}He or thin superconducting films when the field $\theta(\mathbf{u})$ is identified with the phase of the collective wave function. In addition, the elastic energy of Eq. (1) correctly describes liquid crystalline phases for which the bond angle, $\theta(\mathbf{u})$, has periodicity $\frac{2\pi}{p}$ with $p \geq 3$. For a solution of nematigens ($p = 2$) and tilted molecules in a Langmuir film ($p = 1$), two different elastic constants are necessary to account for bend and splay deformations [5], but these are renormalized to the same value at finite temperatures [6]. Besides its experimental significance, the XY model is the cornerstone of our conceptual understanding of topological defects, singular configurations of the field $\theta(\mathbf{u})$.

Like particles, defects have charges and a characteristic Coulomb-like interaction. The charge q, a multiple of $\frac{2\pi}{p}$, can be defined by the amount θ increases along a path enclosing the defect's core. The force between two defects located at positions $\mathbf{u}_i$ and $\mathbf{u}_j$ is determined by the energy stored in the θ field, $E_{\text{int}} = Kq_iq_jU(\mathbf{u}_i, \mathbf{u}_j)$, where the interparticle potential $U(\mathbf{u}_i, \mathbf{u}_j)$ is proportional to the logarithm of the distance in the plane.

On a flat surface, thin layers of superfluids, superconductors, and liquid crystals can all be analyzed within the framework of Eq. (1) [7]. However, there is a crucial difference between, say, the phase of the superfluid order parameter and the angle that describes the local orientation of liquid crystal molecules. The former transforms like a scalar since the quantum mechanical phase does not change when the system is rotated, while the latter represents a vector aligned to the local direction of the molecules. Thus, a common boundary condition for a liquid crystal is for the director to be tangent to the boundary of the substrate. By contrast, no such constraint exists for a ^{4}He film because its wave function is defined in a different space from the one in which the superfluid is confined. This distinction is crucial on a curved surface. In the ground state of a ^{4}He film, the phase $\theta(\mathbf{u})$ is constant throughout the surface and the corresponding energy vanishes. The free energy $\mathcal{F}_s$ to be minimized is a scalar generalization of Eq. (1):

$$\mathcal{F}_s = \frac{K}{2}\int d^2u\sqrt{g}g^{\alpha\beta}\partial_\alpha\theta(\mathbf{u})\partial_\beta\theta(\mathbf{u}). \tag{2}$$

Here the set of coordinates $\mathbf{u} = (u_1, u_2)$ label points on the surface while $\sqrt{g}$ is the determinant of the metric tensor $g_{\alpha\beta}$. On the other hand, a constant bond angle $\theta(\mathbf{u})$ is not the ground state of the liquid crystal because it is measured with respect to an arbitrary basis vector $\mathbf{E}_\alpha(\mathbf{u})$ with $\alpha = 1, 2$. Indeed, it is not possible to make the directions of the molecules parallel everywhere on a curved space; the lowest energy state is attained by optimally distributing the unavoidable bend and splay of the vectors over

the whole surface. The free energy functional $\mathcal{F}_v$ to be minimized is a vector generalization of Eq. (1) [8]:

$$\mathcal{F}_v = \frac{K}{2}\int d^2u\sqrt{g}g^{\alpha\beta}[\partial_\alpha\theta(\mathbf{u}) - \Omega_\alpha(\mathbf{u})][\partial_\beta\theta(\mathbf{u}) - \Omega_\beta(\mathbf{u})], \tag{3}$$

where $\Omega_\alpha(\mathbf{u})$, the connection, compensates for the rotation of the 2D basis vectors $\mathbf{E}_\alpha(\mathbf{u})$ in the direction of u_α. Since the curl of $\Omega_\alpha(\mathbf{u})$ is equal to $G(\mathbf{u})$ [9], the integrand in Eq. (3) cannot be made to vanish on a surface with nonzero Gaussian curvature [$\Omega_\alpha(\mathbf{u})$ is a nonconservative field and hence cannot be equal to $\partial_\alpha\theta$ everywhere]. As the substrate becomes more curved, the energy cost of this geometric frustration can be lowered by generating defects in the ground state even in the absence of topological constraints [10,11].

In this Letter, we introduce a novel coupling between a defect and the varying curvature of the substrate which originates in a conformal anomaly of the free energies of Eqs. (2) and (3). This anomaly arises, even at zero temperature, from imposing a constant cutoff, a, localized at the core of each defect [12]. By contrast, finite temperature conformal anomalies [13] are generated by the presence of a short wavelength cutoff for the fluctuations in $\theta(\mathbf{u})$ at every point on the surface. A physical consequence of the anomalous coupling is that topological defects in superfluids and superconductors interact with the curvature in a radically different way from the case of liquid crystal order [14].

For thin layers of superfluids and superconductors, we prove that the geometric interaction $E^s(\mathbf{u}_i)$ is given by:

$$E^s(\mathbf{u}_i) = -\frac{K}{4\pi}q_i^2 V(\mathbf{u}_i), \tag{4}$$

where $\mathbf{u}_i$ and q_i are, respectively, the position and topological charge of the defect. The geometric potential $V(\mathbf{u})$ satisfies a covariant version of Poisson's equation where the negative of the Gaussian curvature $G(\mathbf{u})$ plays the role of the charge density:

$$D_\alpha D^\alpha V(\mathbf{u}) = G(\mathbf{u}). \tag{5}$$

For an azimuthally symmetric surface such as the bump represented in Fig. 1, we can explicitly obtain $V(\mathbf{u})$, as a function of the radial distance from the top, by employing a two-dimensional analogue of Gauss' law [11]. The resulting potential well $V(r)$ vanishes at infinity and its width and depth are given, respectively, by the linear size of the bump and its aspect ratio squared. Equation (5) has an elegant geometrical interpretation if a set of coordinates is chosen so that the metric tensor is cast in the form $g_{\alpha\beta} = \delta_{\alpha\beta}\exp[-2\omega(\mathbf{u})]$ [8]. The conformal factor, $\omega(\mathbf{u})$ is controlled by the overall shape of the surface and it satisfies the same Poisson Eq. (5) as the geometric potential [8]. We therefore proceed with the identification of $V(\mathbf{u})$ with $\omega(\mathbf{u})$ [15]. This observation will be the basis of our proof of Eq. (4), which results in the novel prediction that a vortex in a superfluid or superconducting film is repelled (attracted) by positive (negative) Gaussian curvature irrespective of its charge and sign.

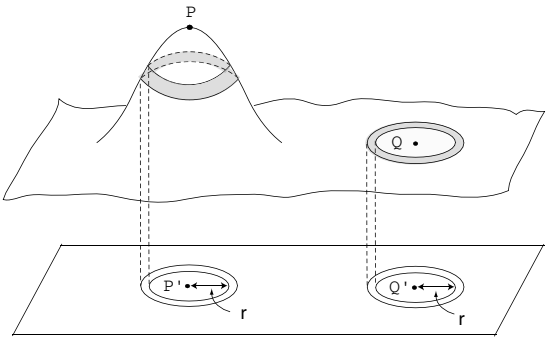

FIG. 1. A corrugated substrate and its downward projection on a flat plane. The shaded strip surrounding P is more stretched than the one surrounding Q despite their projections onto the plane having the same area. The energy stored in the field will be lower if the core of the defect is located at Q rather than P.

For liquid crystals, the geometric interaction $E^v(\mathbf{u}_i)$ contains an additional term discussed in previous investigations of hexatic membranes [17], which arises from the geometric frustration of the vector field. This term, linear in q, happens to contain the same function $V(\mathbf{u})$ as the conformal anomaly of Eq. (4). When both contributions are included, $E^v(\mathbf{u}_i)$ acquires an unexpected dependence on the charge of the defect:

$$E^v(\mathbf{u}_i) = Kq_i\left(1 - \frac{q_i}{4\pi}\right)V(\mathbf{u}_i). \tag{6}$$

The interpretation of $V(\mathbf{u})$ as a geometric potential and the linear dependence on q in the first term of Eq. (6) are consistent with the general belief that a defect interacts logarithmically with the Gaussian curvature, as an electrostatic particle would with a background charge distribution. However, $E^v(\mathbf{u}_i)$ does not grow linearly with the charge of the defect, as expected from the electrostatic analogy. Instead, the geometric interaction peaks for a defect of charge 2π and eventually becomes repulsive for q greater than the critical charge $q_c = 4\pi$ [18].

The quadratic coupling has an intuitive explanation in the case of azimuthally symmetric surfaces. Consider a very thin superfluid film deposited on the surface illustrated in Fig. 1 with a vortex of charge q placed on top of the bump. In order to calculate the energy stored in the field, we only need to know that the superfluid phase $\theta(\mathbf{u})$ changes uniformly by q along a circumference of length $2\pi r$ centered on the defect. Inspection of Eq. (2) reveals that the energy density of the field in the shaded strip at distance r is proportional to $(\frac{q}{r})^2$, where r is the distance to the singularity measured in the plane of projection (see Fig. 1). By vertically stretching the surface, the amount of area in the shaded strip is increased with respect to its projection on the plane, while the energy density is un-

changed. As a result, the total energy stored in the field is greater when a vortex sits on top of a bumpy surface than when the same vortex is located at the center of a flat disk of the same area. Hence, it is energetically favorable for the vortex to migrate to the flat portions of the surface. In this case, the vortex is far away from the bump so that the total energy stored in the field does not differ much from the flat plane result [19]. For less symmetric surfaces, the resulting geometric interaction will depend on the shape of the entire surface as embedded in the metric tensor.

The physical origin of the *linear* coupling between defects and curvature in Eq. (6) is illustrated in Fig. 2 for a disclination of charge 2π centered on a bump. As the curvature of the bump is increased, the bend or splay of the director of the liquid crystal decreases and hence the energy stored in the vector field is reduced. As a result, this linear coupling causes positively (negatively) charged defects to be attracted by positive (negative) Gaussian curvature [17]. However, this mechanism competes with the repulsive geometric interaction illustrated in Fig. 1 that is at work also in the case of liquid crystal order. We note that the linear coupling is absent for superfluids because, in Eq. (2), $\partial_\alpha \theta(\mathbf{u})$ is not coupled to a curvature dependent connection, $\Omega_\alpha(\mathbf{u})$, as it is in Eq. (3).

The critical value $q_c = 4\pi$, where the single defect potential $E^v(\mathbf{u}_i)$ changes sign, can be determined from simple geometrical arguments. Consider an isolated disclination of charge q on a hemispherical cup placed on a flat plane. On account of azimuthal symmetry, the force acting on the defect depends *only* on the net Gaussian curvature enclosed by the circle on which it is placed, see Fig. 3(a) [11]. This interaction is unchanged if we deform the outer region of the plane and eventually compactify it to form a sphere as illustrated in Fig. 3(b). In order to satisfy topological constraints [20], we still need to place a shadow defect of charge $(4\pi - q)$ at the south pole (the only position outside the circle that does not destroy the azimuthal symmetry of the initial problem). The curvature-defect interaction on the hemisphere is thus reduced to the well known defect-defect interaction on the sphere [21]. The latter is proportional to $q(4\pi - q)$ and so is the curvature-defect interaction on the deformed plane of Fig. 3(a), in agreement with Eq. (6). This provides evidence that a disclination of charge greater than 4π will be repelled from regions of positive curvature.

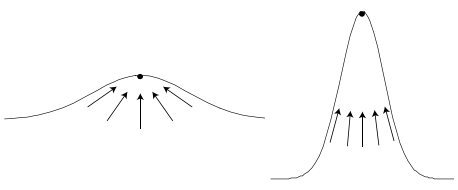

FIG. 2. Disclinations of charge 2π located on top of bumps with different aspect ratios. The amount of splay in the liquid crystal director on the taller bump is reduced and hence the energy density is lower.

We now present a derivation of the coupling between curvature and defects in helium and superconducting films that employs the method of conformal mapping, often adopted in electromagnetism and fluid mechanics to simplify the boundary of complicated planar regions. In this context, we use conformal mappings to relate the complex task of finding the field energy on an arbitrarily deformed target surface to an equivalent problem on a homogeneous reference surface (see Fig. 4). A conformal mapping has two equivalent defining properties: angles map to equal angles, and very small figures map to figures of nearly the same shape. One can always find a conformal mapping from the target to the reference surface [8] such that $g_T = e^{-2\omega(\mathbf{u})} g_R$, where g_T and g_R are the metric tensors on the target and reference surfaces, respectively. The scaling factor $e^{\omega(\mathbf{u})}$ varies with the position $\mathbf{u}$ on the target surface, so that larger figures are inhomogeneously distorted when they are mapped from the target to the reference surface. We choose the reference surfaces to be undeformed and of the same topology as the target spaces (e.g., $g_R = \delta_{\alpha\beta}$ for a corrugated plane). Defects on the target surface are mapped onto a set of "image defects" on the reference surface.

The crucial property of the scalar free energy $\mathcal{F}_s$ is its invariance under the rescaling of the metric by the conformal factor [22]. However, the conformal symmetry of $\mathcal{F}_s$ is broken upon introducing a short distance cutoff a that is necessary to prevent the energy from diverging in the core of the defect. Because of the varying scaling factor, the constant physical core radius a is stretched or contracted when projected on the reference space by an amount dependent on the position of the defect (see Fig. 4). The radius of the image of the i^{th} core is $a_i = e^{\omega(\mathbf{u}_i)} a$. It is this conformal anomaly that is responsible for generating the geometric interaction in Eq. (4). In fact, the energy of the defects in the target space E_T is equal to the energy of a configuration of defects (on the reference surface) whose core radii are position dependent. This problem can be further transformed into the simpler task of finding the energy E_R for a set of interacting defects with constant core radius a plus an effective geometric potential that accounts for the variation of the core size with position. This geometric potential can be derived with the aid of Fig. 4. If a_i is smaller (larger)

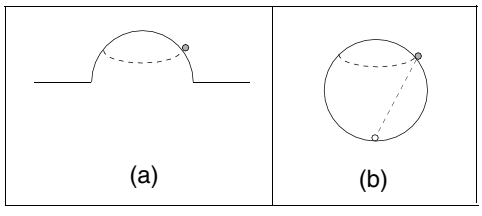

FIG. 3. (a) An isolated disclination on a deformed plane feels a force that depends only on the enclosed Gaussian curvature. (b) The deformed plane is compactified to the sphere by placing a shadow defect at the south pole.

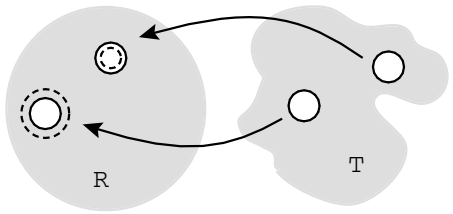

FIG. 4. Conformal mapping of the target surface T onto the reference space R. The continuous disks on both surfaces represent the "physical" cores of constant radius a. The dashed lines represent the position-dependent images on R of the defect cores on T with variable radii a_i. Note that the energy stored in the annuli comprised by the dashed and continuous lines in R must be added or subtracted to E_R to obtain E_T.

than a, the energies stored in the annular regions indicated in Fig. 4 need to be added (subtracted) from E_R to obtain E_T. To calculate this extra energy, we introduce a set of polar coordinates (r, ϕ) centered on the i^{th} defect. Near the defect of charge q_i, the phase is given by $\theta \approx \frac{q_i}{2\pi}\phi$ and the energy density is $\frac{Kq_i^2}{8\pi^2 r^2}$. Upon integrating it over the annulus comprised between a and $a_i = e^{\omega(\mathbf{u}_i)}a$ (see Fig. 4), we obtain

$$E_T - E_R = -K\sum_{i=1}^{N_d}\frac{q_i^2}{4\pi}\omega(\mathbf{u}_i), \tag{7}$$

where N_d is the number of defects. The energy E_R accounts for defect-defect interactions since any potential felt by a single defect would have to be constant because all points are equivalent on the reference surface (undeformed sphere or plane). Recalling that $\omega(\mathbf{u}) = V(\mathbf{u})$, we recover the result of Eq. (4) with no dependence on the microscopic physics because the core size a drops out in Eq. (7) [16]. In the case of liquid crystal order, the contribution of the anomaly is simply added to the term linear in q as indicated in Eq. (6) [11].

Experiments that test our predictions can be realized by coating a bump with a thin layer of superfluid helium and rotating it around its axis of symmetry so that a single vortex forms [23]. The competition between the (repulsive) geometric interaction and the confining parabolic potential (generated by the rotation) would cause the equilibrium position of the vortex to shift from the center of the bump if its height exceeds a critical value. The vortex line could be detected by trapping of electrons on its core [24]. Other experiments may detect an inhomogeneous distribution of thermally induced defects resulting from the combined effect of the anomalous coupling and the dependence of their Coulomb-like interaction on the varying curvature.

We have demonstrated that the interaction between defects and curvature in 2D XY-like models depends crucially on the nature of the underlying order parameter and we have shown how to explicitly derive the resulting geometric force from the shape of the surface.

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