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Citation

Upadhyaya, N., & Vitelli, V. (2011). Quantum buckling. *Physical Review E*, 84(4), 040601(R).
doi:10.1103/PhysRevE.84.040601

Version: Not Applicable (or Unknown)

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Downloaded from: <https://hdl.handle.net/1887/61363>

Note: To cite this publication please use the final published version (if applicable).

Quantum buckling

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(Received 30 June 2011; revised manuscript received 2 September 2011; published 10 October 2011)

We study the mechanical buckling of a freestanding superfluid layer. A topological defect in the phase of the quantum order parameter distorts the underlying metric into a surface of negative Gaussian curvature, irrespective of the sign of the defect charge. The resulting instability is in striking contrast with classical buckling, where the in-plane strain induced by positive (negative) disclinations is screened by positive (negative) curvature. We derive the conditions under which the quantum buckling instability occurs in terms of the dimensionless ratio between superfluid stiffness and bending modulus. An ansatz for the resulting shape of the buckled surface is analytically and numerically confirmed.

DOI: [10.1103/PhysRevE.84.040601](https://doi.org/10.1103/PhysRevE.84.040601)

PACS number(s): 67.80.dm, 46.32.+x, 67.10.Hk, 67.80.dj

The rapid trend toward the miniaturization of electromechanical systems has spurred a flurry of theoretical activity aimed at investigating quantum mechanical effects in the context of more classical subjects such as heat transfer and mechanical stability [1,2]. Common building blocks for these devices are carbon-based materials such as nanotubes and graphene, essentially two-dimensional elastic sheets which are often bent or wrinkled [3–7]. Much effort has been directed toward understanding how quantum surface states are affected by the underlying curvature of these spaces [8–12]. However, less attention has been devoted to the converse problem: Can quantum mechanical effects modify the shape and mechanical stability of nanostructures?

These questions have so far been relegated to the fringe of mainstream engineering applications, since it is challenging to probe experimentally the regime where the characteristic energy of quantum effects is comparable to the bending energy. Furthermore, the interplay between a quantum order parameter and geometry is a more subtle theoretical problem than its classical counterpart. Quantum mechanical degrees of freedom *live* in an internal space distinct from the local tangent plane of the underlying substrates. As a result, coupling mechanisms between the in-plane quantum order parameter and curvature are typically less intuitive. By contrast, classical buckling is the paradigmatic example of how elastic stresses in a crystal or liquid-crystal monolayer are *screened* by curvature [13–22].

In this Rapid Communication, we demonstrate a quantum analog of buckling and trace its distinctive physical and mathematical origins. Specifically, we consider the two-dimensional (2D) order parameter $\psi(\rho) = |\psi|e^{i\theta(\rho)}$ that describes superfluid or superconducting phases of a quantum condensate and show that the presence of isolated vortices or antivortices can buckle a thin layer of freely suspended superfluid. However, there is a crucial qualitative difference between this phenomenon and classical buckling, as summarized pictorially in Fig. 1. Classical buckling requires that positive (negative) disclinations induce buckling of the monolayer into conical singularities of positive (negative) Gaussian curvature [23–25]. Screening requires that the sign of the defect charge is matched by the sign of the curvature; see Figs. 1(a) and 1(b). In contrast, our stability analysis reveals that (despite the lack of an explicit defect screening mechanism) vortices and antivortices in a quantum order parameter can induce buckling of a superfluid

layer into a conical singularity of negative Gaussian curvature, independently of the sign of the defect charge; see Figs. 1(c) and 1(d). Previous studies of the energetics of topological defects on *rigid* surfaces [10,15] do not allow us to deduce if and how a *soft* substrate will deform in the presence of defects. In order to assess under what conditions buckling occurs and what the resulting shape is, we perform a detailed variational analysis to minimize both the in-plane and bending energies, and propose an experimental realization of this quantum buckling effect.

Consider for simplicity a flexible freestanding layer of superfluid. If surface tension can be ignored, the total energy functional H is given by the sum of the bending energy H_κ ,

$$H_\kappa = \frac{\kappa}{2} \int d^2\mathbf{u} \sqrt{g} M^2(\mathbf{u}), \quad (1)$$

and the condensate kinetic energy H_v ,

$$H_v = \frac{K}{2} \int d^2\mathbf{u} \sqrt{g} g^{\alpha\beta} \partial_\alpha \theta(\mathbf{u}) \partial_\beta \theta(\mathbf{u}). \quad (2)$$

Here, $\mathbf{u} = \{u^1, u^2\}$ is a set of two-dimensional coordinates specifying positions $\mathbf{R}(\mathbf{u})$ in the plane of the surface, $g_{\alpha\beta} = \partial_\alpha \mathbf{R} \cdot \partial_\beta \mathbf{R}$ and $g = \det(g_{\alpha\beta})$ denote the metric tensor and its determinant, $M(\mathbf{u})$ is the mean curvature [26], κ is the bending rigidity, $K = \rho_s \hbar^2 / 2m_s^2$ is the superfluid stiffness constant given in terms of the atomic mass m_s and density ρ_s of the superfluid, and $\partial_\alpha \theta(\mathbf{u})$ gives the local superfluid velocity.

In order to grasp intuitively the origin of the quantum buckling instability, consider Eq. (2) for the case of an isolated vortex of topological charge $q = \pm 1$ at the tip of a conical singularity: an azimuthally symmetric surface denoted by a height function (out of plane shift) $h(\rho, \phi) = m\rho$, where we have used 2D polar coordinates $\mathbf{u} = \{\rho, \phi\}$. Note that the Gaussian curvature for this surface is a delta function that vanishes everywhere except at the tip of the cone. Due to the azimuthal symmetry, we expect the elastic variable $\theta = q\phi$ to retain its flat space form, so that $\nabla\theta = \frac{q}{\rho}\hat{\mathbf{e}}_\phi$, where $\hat{\mathbf{e}}_\phi$ is the angular unit vector in polar coordinates. With the metric expressed in terms of the slant length of the cone $l = \sqrt{1 + m^2}\rho$, we can evaluate Eq. (2) to obtain

$$E_v = \pi K q^2 \sqrt{1 + m^2} \ln \left(\frac{R}{a_0} \right), \quad (3)$$

FIG. 1. (Color online) Illustrative plots for surface buckling corresponding to (a) positive disclination, (b) negative disclination, (c) vortex, and (d) antivortex. Positive (negative) topological defects are shown with red (yellow) dots, where a positive (negative) disclination is screened by a surface with positive (negative) Gaussian curvature in the top row, while a vortex (antivortex) buckles the underlying metric into a negative Gaussian curvature surface in the bottom row.

where, a_0 is a microscopic cutoff length (of the order of the vortex core radius) and $R \gg a_0$ is the size of the membrane. We see that the energy required for the vortex (antivortex) to occupy the tip of a conical singularity is always greater than its flat-space counterpart by a positive definite factor $\sqrt{1+m^2}$ in Eq. (3). The comparison is meaningful in our assumed limit $R \rightarrow \infty$ where one does not need to worry about measuring the size of the cone along itself or on its base. This simple calculation demonstrates that it is not energetically favorable for the vortex to buckle the substrate into a surface with a positive delta Gaussian curvature [the positive definite bending energy in Eq. (1) only adds an extra penalty].

Contrast the result obtained in Eq. (3) with the corresponding one for a liquid-crystal membrane. In the liquid-crystal case, the order parameter θ describes the orientation of a vector, not the (scalar) phase of a wave function. This distinction implies that the elastic variable θ must explicitly couple with the underlying curvature and thus each instance of $\partial_\alpha \theta$ in Eq. (2) appears in the form $\partial_\alpha \theta - A_\alpha$, where the connection A_α is a geometric gauge field whose curl equals the Gaussian curvature [26]. As a result of this difference, the leading order correction in m appears with a minus sign in Eq. (3) and it can be sufficiently large to overcome the bending energy cost [23,24]. This is the mathematical mechanism responsible for the classical buckling of liquid-crystal as well as crystalline membranes: The geometric gauge field couples elastic defects to Gaussian curvature via cross terms in $(\partial_\alpha \theta - A_\alpha)^2$, thereby providing a direct mechanism for screening the defect charge.

Can there be buckling in the absence of a geometric gauge field? In order to answer this question, we take a more systematic and versatile approach to track the curvature correction estimated in Eq. (3). For general surfaces, the vortex self-energy is the sum two contributions, $E_v = E_f + E_s$, where E_f is the flat-space energy of the vortex and $E_s = -Kq^2 V(\mathbf{u})$ is expressed in terms of the geometric potential

$V(\mathbf{u})$ that satisfies a covariant form of Poisson's equation:

$$D_\alpha D^\alpha V(\mathbf{u}) = G(\mathbf{u}). \quad (4)$$

Here, the negative of the Gaussian curvature $G(\mathbf{u})$ plays a role analogous to the electrostatic charge density [10,11]. The geometric potential in Eq. (4) arises from evaluating with conformal mappings the Green's function of two-dimensional electrostatics on a curved surface. Note, however, that the domain of integration in Eq. (2) must be punctured around the defect cores which introduces a small length of order a_0 that breaks the conformal invariance of the Hamiltonian and generates the additional coupling $V(\mathbf{u})$ between vortices and curvature. This contribution is an example of a conformal anomaly because it is independent of the length a_0 responsible for breaking the conformal symmetry [31].

Equation (4) can be readily solved for a family of surfaces whose height function is described by $h(\rho, \phi) = \rho f(\phi)$. The geometric potential for a singular distribution of Gaussian curvature reads

$$V(\rho) = -2\pi s \Gamma(\rho + a_0, \rho), \quad (5)$$

where the integrated Gaussian curvature s can be obtained using the Gauss-Bonnet theorem [23],

$$s = 1 - \frac{1}{2\pi} \int_0^{2\pi} d\phi \frac{[1 + f'^2(\phi) - f(\phi)f''(\phi)]}{[1 + f'^2(\phi) + f^2(\phi)]^{1/2}[1 + f'^2(\phi)]},$$

and the Green's function Γ evaluated at the core of the defect takes the form $\Gamma(\rho + a_0, \rho) = \lim_{\rho \rightarrow a_0} -A(\ln \frac{\rho}{a_0} - \ln \frac{R}{a_0}) = A \ln \frac{R}{a_0}$ [32]. The coefficient A is then given by [23]

$$A = \left[\int_0^{2\pi} d\phi \frac{1 + f'^2(\phi)}{[1 + f^2(\phi) + f'^2(\phi)]^{1/2}} \right]^{-1}. \quad (6)$$

Here, primes denote derivatives with respect to ϕ . Adding the flat-space energy $E_f = \pi K q^2 \ln \frac{R}{a_0}$ to the self-energy $E_s = -\pi K q^2 V = 2\pi^2 K q^2 A s \ln \frac{R}{a_0}$, we obtain the total vortex energy for a singular distribution of Gaussian curvature

$$E_v = \pi K q^2 (1 + 2\pi A s) \ln \left(\frac{R}{a_0} \right). \quad (7)$$

As a check, upon evaluating Eq. (7) for a simple cone (positive delta Gaussian curvature) described by $f(\phi) = m$, $A = \frac{\sqrt{1+m^2}}{2\pi}$, and $s = 1 - \frac{1}{\sqrt{1+m^2}}$, we recover the result obtained in Eq. (3).

Next, consider a saddle: a surface with negative delta Gaussian curvature. We take the simplest surface described by a height function, $h(\rho, \phi) = m\rho \cos(2\phi)$. The derivation for the total vortex energy proceeds exactly as outlined above, substituting for $f(\phi) = m \cos(2\phi)$ into the general expressions obtained in Eqs. (6) and (7). Further, the bending energy can be evaluated from Eq. (1) where, for our assumed height function, the mean curvature takes the form [24]

$$M = \frac{[1 + f^2(\phi)][f(\phi) + f''(\phi)]}{2\rho[1 + f^2(\phi) + f'^2(\phi)]^{3/2}}. \quad (8)$$

Since this surface is not azimuthally symmetric, the resultant expressions can only be expressed as integrals over ϕ . However, restricting ourselves to small deviation from flatness, i.e., $m < 1$, we can expand H_κ , A , and s in a perturbation

FIG. 2. (Color online) Normalized energy $E(m) = E/[(\pi K \ln(\frac{R}{a_0}))]$ as a function of parameter m^2 for $r = \frac{4}{3}r_c$ (small dots black), $r = r_c$ (solid line black), $r = \frac{3}{4}r_c$ (solid red), $r = \frac{1}{2}r_c$ (dash-dot green), and $r = \frac{2}{5}r_c$ (dot blue), where $r_c \sim 0.17$ is the critical ratio of bending rigidity κ to superfluid stiffness K , below which the substrate can buckle. For $r < r_c$, the normalized energy curves show a minima below 1 (top). Bottom plot shows $E(m^*)$ as a function of r also for the saddle surface, where m^* is the value of m for which $E(m)$ has a minimum. The plateau for $r > r_c = 0.17$ shows that the substrate cannot buckle for a ratio higher than the critical value.

series in m and integrate the resulting expressions to obtain the following form, correct to order $O(m^2)$, for the combined bending and vortex energies:

$$E = \pi K q^2 \left[1 + \left(\frac{9}{2}r - \frac{3}{4} \right) m^2 + O(m^4) \right] \ln \left(\frac{R}{a_0} \right). \quad (9)$$

Here, we have introduced a dimensionless parameter $r = \frac{\kappa}{K}$ that serves to quantify the competition between the condensate kinetic energy and bending energy. Inspection of Eq. (9) reveals a critical $r_c \sim \frac{1}{6}$, below which the total energy of the buckled substrate ($m \neq 0$) is less than its flat counterpart ($m = 0$). Further, due to the quadratic dependence on defect charge q , this result is independent of the sign of the vortex defect. Hence both vortices and antivortices will distort the underlying metric into a saddle shape.

In order to determine the shape of the buckled substrate, we expand the total energy E in Eq. (9) to order $O(m^6)$ and find m^* corresponding to its minimum. In Fig. 2, we plot the total energy E so obtained, normalized by $\pi K \ln(\frac{R}{a_0})$, against the parameter m for different choices of r . As the ratio is decreased below the critical value $r_c = 0.17$, the energy (corresponding to red, green, and blue curves) has a minimum at m^* indicating that buckling of the underlying substrate into a saddle shape is energetically favorable.

We next test the validity of our ansatz for the shape of the buckled substrate by expressing the height function $h(\rho, \phi) = \rho \sum_i [a_i \cos(2i\phi) + b_i \sin(2i\phi)]$, in the form of a truncated Fourier series. Thus, we numerically seek the coefficients

$\{a_i, b_i\}$ that minimize the total Hamiltonians appearing in Eqs. (1) and (2) by approximating integrals with finite sums. Note that the height function used in the perturbation expansion method corresponds to retaining just the first term a_1 in this series. The lower panel in Fig. 2 shows the energy so obtained as a function of r , where we have used the notation $E(m^*)$ to denote the energy obtained by solving for the Fourier coefficients that minimize the Hamiltonians even if we are using more than one term in the Fourier series expansion. Above r_c , the total energy remains constant, indicating that for a large ratio there is no choice of coefficients that minimizes the total energy and, therefore, buckling is not favorable. However, below r_c , the total energy decreases as r is reduced, thus confirming for both a vortex and an antivortex the buckling of the underlying substrate into a saddle with the dominant contribution to the energy coming from only the first term in the Fourier series, in agreement with our analytical ansatz.

Although classical screening of defects by curvature of matching sign is absent for the condensate, inspection of Eq. (9) suggests that the reduced vortex energy E (dressed by bending contributions) can lower the critical temperature T_c for the Kosterlitz-Thouless transition on a flexible substrate. This is apparent from estimating T_c by balancing the vortex energy with its entropy S [27]. For a two-dimensional substrate of size R , the number of possible positions of a vortex is still proportional to $(\frac{R}{a_0})^2$, as in flat space. Any geometric corrections are subleading in the limit of a large system size and one recovers the familiar result $S \approx k_B \ln(\frac{R}{a_0})^2$, where k_B is the Boltzmann constant. By contrast, the deformation of the underlying metric ($m \neq 0$) changes the prefactor of the logarithmic divergence of the energy E in Eq. (9). At the transition, the free energy $F = E - T_c S$ vanishes, leading to a reduced critical temperature $T_c = \frac{E}{2k_B \ln(R/a_0)}$. For instance, if the bending rigidity is below the critical value so that $r = \frac{1}{2}r_c$, we can read off from the inset of Fig. 2 the corresponding shape of the saddle $m^2 \sim 0.21$ yielding $T_c \sim \frac{0.47K}{\pi k_B}$, whereas for a flat substrate with $m = 0$, the corresponding temperature will be $T_c \sim \frac{0.50K}{\pi k_B}$, with K/k_B of the order of 40 K for a superfluid film of thickness around 100 Å.

As an experimental realization, consider a thin layer of superfluid helium on a cesium-coated surface with a circular orifice of radius R . The choice of cesium ensures that the interaction with the substrate is such that the layer can be freely suspended on the orifice [28]. The gravitational energy $gR^3\rho_s$ is then negligible compared to the characteristic energy K driving the quantum buckling, provided that the orifice is engineered on submicron scales.

To conclude, we have demonstrated how in-plane quantum order can deform a soft substrate and induce buckling of a vortex even in the absence of screening between its topological charge and curvature. Possibilities for future work could include studying the effect of multiple interacting defects and the resultant formation of ripples on freestanding membranes [29,30].

We thank A. Turner, A. Achucarro, A. Boyarsky, L. Gomez, W. T. M. Irvine, L. Rademaker, and W. van Saarloos for helpful discussions. N.U. gratefully acknowledges financial support from the Stichting voor Fundamenteel Onderzoek der Materie (FOM).

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