Free energies of isolated five- and sevenfold disclinations in hexatic membranes

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We examine the shapes and energies of five- and sevenfold disclinations in low-temperature hexatic membranes. These defects buckle at different values of the ratio of the bending rigidity κ to the hexatic stiffness constant K_A suggesting *two* distinct Kosterlitz-Thouless defect proliferation temperatures. Sevenfold disclinations are studied in detail numerically for arbitrary κ/K_A. We argue that thermal fluctuations always drive κ/K_A into an unbuckled regime at long wavelengths, so that disclinations should, in fact, proliferate at the *same* critical temperature. We show analytically that both types of defects have power law shapes with continuously variable exponents in the unbuckled regime. Thermal fluctuations then lock in specific power laws at long wavelengths, which we calculate for five- and sevenfold defects at low temperatures.

I. INTRODUCTION

Topological defects, such as dislocations and disclinations, behave differently in membranes and monolayers. Monolayers are films, typically with a triangular lattice in their low-temperature crystalline phase, strongly confined to a plane by, for example, surface tension. In monolayers, pointlike topological imperfections are the ingredients of a detailed two-stage melting theory [1,2], which predicts that the usual latent heat associated with a first-order melting transition can be spread out over an intermediate hexatic phase characterized by long-range bond orientational order and short-range positional order [2,3]. In contrast to monolayers, membranes can easily buckle out of the two-dimensional plane. This buckling lowers defect energies. The standard example of a membrane is an extended lipid bilayer surface in water solution [4]. Dislocation energies in membranes are finite, in contrast to a logarithmic divergence with system size for monolayers, which leads to melting of crystalline membranes at any nonzero temperature for entropic reasons [5,6]. The generic low-temperature phase for membranes at large enough length scales is inevitably a hexatic liquid with long-range bond orientational order and a vanishing shear modulus.

Disclinations can also lower their energy by buckling. The energy of a single disclination in an otherwise crystalline monolayer diverges with the square of the system size. Buckling in a membrane leads to energies of plus and minus disclinations that diverge only logarithmically with size [5]. Interestingly, the coefficients of these logarithmic divergences are different: the energy of fivefold (plus) disclinations is about a factor of 2 lower than that of sevenfold (minus) ones [6]. This asymmetry differs from the behavior of defects in most monolayer materials that exhibit the Kosterlitz-Thouless defect unbinding transition [2]. Plus and minus vortices in superfluid helium films, for example, must have ex-

actly the same core energies and logarithmic divergences with system size by time reversal invariance. Equality of energies also holds for dislocations with equal and opposite Burgers vectors in crystalline monolayers. Plus and minus disclinations in hexatic monolayers have different core energies, due to the different local environments of the five- and sevenfold defects, but the coefficients of their logarithmically diverging energies are identical [1]. Identical coefficients for the logarithmically diverging ± defect pairs ensure that the elementary Kosterlitz-Thouless energy-entropy balance leads to the same proliferation temperature for each type of defect. This famous argument [7] predicts that five- or sevenfold defects proliferate whenever the free energy to create a disclination, $F_5(R) = E_5(R) - 2k_BT \ln(R/a_0)$ or $F_7(R) = E_7(R) - 2k_BT \ln(R/a_0)$, becomes negative. Here $E_5(R)$ and $E_7(R)$ are disclination energies as a function of the system size R, and a_0 is a microscopic cutoff.

The disparate disclination energies in buckled crystalline membranes suggest that these energies may also differ in hexatic membranes, as recently emphasized by one of us [8]. The energy of fivefold disclinations in hexatic membranes has been studied by Seung [9], Guitter [10], and Guitter and Kardar [11]. The results depend on two dimensionless parameters, κ/k_BT and K_A/k_BT, where κ and K_A are the membrane bending rigidity and hexatic stiffness constant, respectively. When $\kappa/K_A \gg 1$, the membrane remains asymptotically flat in the presence of both five- and sevenfold defects, and the energies diverge logarithmically with equal coefficients. When $\kappa/K_A < 11/72$, however, the fivefold disclination buckles and reduces its in-plane bond angle energy at the expense of bending energy. The resulting energy still diverges logarithmically, but the coefficient is reduced by buckling. The locus of Kosterlitz-Thouless transition temperatures for fivefold defects in membranes when buckling is included is shown by the solid curve in Fig. 1. These disclinations assume a conical shape when $\kappa/K_A < 11/72$ and, as shown in Sec. III, exhibit a weaker
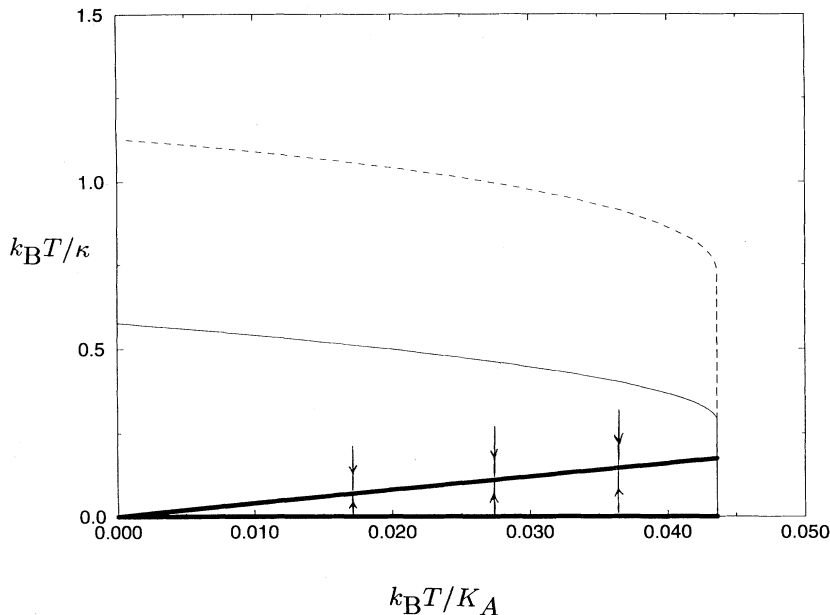
FIG. 1. Phase diagram for proliferation of isolated fivefold (solid curve) and sevenfold (dashed curve) disclinations. Five- and sevenfold disclinations buckle above lines (not shown) extending from the origin to the tops of the vertical portions of the solid and dashed curves, respectively. For small κ or K_A (outside the curves), disclinations proliferate. Lines of renormalized effective rigidities are also indicated (bold). Renormalization group flows obtained by David et $al.$ in a low-temperature perturbation expansion away from the unstable fixed line at $\kappa = \infty$ to the stable line describing the crinked phase are indicated by the arrows.

power law deviation from flatness when $\kappa/K_A > 11/72$, with continuously variable exponents.

In this paper, we study sevenfold defects and determine the curve for their proliferation, shown as the dashed curve in Fig. 1. Because buckled sevenfold defects do not have the azimuthal symmetry of fivefold defects, some numerical work is necessary. As anticipated in [8], the sevenfold hexatic disclination energy exceeds its fivefold counterpart for $\kappa/K_A \ll 1$, leading to a larger Kosterlitz-Thouless critical temperature. We find that sevenfold disclinations buckle to reduce the coefficient of their logarithmically diverging energy whenever $\kappa/K_A < 13/216$, while they remain asymptotically flat when κ/K_A exceeds this value. There is again a power law deviation from flatness for $\kappa/K_A > 13/216$. As is evident from Fig. 1, a naive application of the Kosterlitz-Thouless criterion to hexatic membranes leads to two distinct defect proliferation temperatures over a significant range of parameters.

Our results provide useful information about deformations of hexatic membranes near defects at relatively low temperatures. However, understanding the behavior at very large distances from the defect cores requires that we take into account the nonlinear renormalization of κ and K_A by thermal fluctuations. These effects were first studied in a perturbative, low-temperature expansion by David et $al.$ [12], who found that the hexatic phase of membranes is controlled by a line of fixed points in the $(k_BT/K_A, k_BT/\kappa)$ plane with slope $\kappa^*/K_A^* = 1/4$. The parameters κ and K_A are driven toward the fixed line by thermal fluctuations even if they initially lie in one of the buckled regimes. This line and the associated nearby renormalization group flows are indicated by the heavy curve in Fig. 1. The unstable Kosterlitz-Thouless fixed line for hexatic monolayers ($\kappa \to \infty$) is also shown. Because the stable fixed line has a slope far below the crit-

ical slopes for buckling of five- or sevenfold disclinations, we conclude that these defects probably have symmetrically diverging energies when thermal fluctuations are taken into account. Provided that the line of stable fixed points, which is only known perturbatively at low temperatures [12], does not bend significantly before piercing the vertical part of the Kosterlitz-Thouless instability curve, both defects will remain unbuckled and proliferate at the same point. Although the coefficients of the logarithmic divergences in five- and sevenfold disclination energies are the same, these defects have interesting power law shapes in the "unbuckled" regime.

Park and Lubensky have recently incorporated fluctuations in the internal metric of the membrane into the work of David et $al.$ [13]. Inclusion of these fluctuations appears to be necessary to account for local in-plane shear and compression modes, whose primary effect is to dilate and reshuffle the nearest-neighbor bond connectivity of the atomic or molecular constituents. Averaging over these modes leads to an $effective$ coupling K_A^{eff}, which should replace the hexatic stiffness in the model used here. The bending rigidity is unchanged. The remaining renormalization of κ and K_A^{eff} by thermal undulations, however, is identical to that found by David et $al.$ [12]. Thus our overall conclusions are unchanged, provided that we use κ and the renormalized coupling K_A^{eff} in our results and in Fig. 1. In agreement with the results of the study of disclination statistical mechanics by Park and Lubensky [13], we still expect a symmetrical $\pm$ disclination unbinding transition with unbuckled defects in hexatic membranes. Disclinations cannot unbind separately, in contrast to the predictions of the "naive" Kosterlitz-Thouless argument, provided that the thermal renormalization of the ratio κ/K_A^{eff} to $1/4$ at long wavelengths remains intact out to the transition temperature [15].

In independent work, Park and Lubensky have also studied the buckling of sevenfold disclinations [14]. Their result for the critical ratio κ/K_A and the behavior near the buckling transition are in agreement with the results presented here. Our results are more reliable in the limit $\kappa/K_A \gg 1$, however.

It is worth noting that similar issues involving disclination asymmetry arise even for monolayers, when two-dimensional nematic order is present. The topologically stable defects are now $\pm 1/2$ disclinations and the ordered state is described by both bend and splay elastic constants K_1 and K_3 [16]. When $K_1 \neq K_3$, the energies of $\pm$ disclinations again diverge logarithmically with different coefficients. Here a renormalization group analysis of nonlinear effects due to thermal fluctuations shows that K_1 and K_3 are driven to equality at long wavelengths, so that the "one-Frank-constant approximation" becomes asymptotically correct at long wavelengths [17]. The disclinations energies are equal in this limit and one again expects a symmetrical defect unbinding transition [18].

We should stress that even though disclination energies are asymptotically symmetrical in hexatic membranes, buckling will still occur locally for appropriate parameter values. Buckling will persist out to length scales such that the renormalized value of the ratio $\kappa/K_A^{\rm eff}$ is in the unbuckled regime. An intrinsic microscopic asymmetry, moreover, can still arise in the liquid, after the disclinations unbind. As emphasized in Ref. [9], a net excess of disclinations should have important consequences in liquid membranes with free boundary conditions or a topology that can change on experimental time scales. Exactly how the $\pm$ disclination populations become identical as one approaches the liquid-to-hexatic transition from the liquid phase is an interesting topic for future research.

In Sec. II we discuss how membrane buckling can screen disclinations. In Sec. III we review analytical calculations of the energy of a fivefold disclination. We use approximate theory and exact numerical calculations to calculate the energy and shape of a sevenfold disclination in Sec. IV. We review the important effects of thermal fluctuations, including how these fix the asymptotic defect shapes in the unbuckled regime, in Sec. V.

II. CURVED HEXATIC MEMBRANES WITH DEFECTS

The Hamiltonian for a flexible, hexatic membrane is given in the limit of vanishing surface tension by [5,19]

$$H = H_\theta + H_\kappa + H_{\bar{\kappa}},$$
$$H_\theta = \frac{K_A}{2} \int d^2 S (\partial_i \theta - \Omega_i) g^{ij} (\partial_j \theta - \Omega_j),$$
$$H_\kappa = \frac{\kappa}{2} \int d^2 S \bar{H}^2,$$
$$H_{\bar{\kappa}} = \bar{\kappa} \int d^2 S K . \tag{1}$$

All these integrals are over the surface of the membrane. For the case of a membrane with free boundary conditions there should also be line tension and geodesic curvature terms. We neglect these terms. Here g^{ij} is the inverse metric tensor, $\bar{H}$ is the mean curvature, K is the Gaussian curvature, and the gauge field is defined by $K = \gamma^{ij} D_i \Omega_j$. Upon defining $g = \det(g_{ij})$, we have $\gamma^{ij} = \epsilon_{ij} g^{-1/2}$ with $\epsilon_{11} = \epsilon_{22} = 0$ and $\epsilon_{12} = -\epsilon_{21} = 1$. The surface area element is given by $d^2 S = d^2 \sigma g^{1/2}$.

We are interested in very flexible membranes, as opposed to monolayers, and so we will neglect the possible surface tension term of the form $H_r = r \int d^2 S$. We will also ignore the Gaussian curvature term $H_{\bar{\kappa}}$, which is a perfect derivative by the Gauss-Bonnet theorem. H_κ is the standard bending energy term and H_θ is the contribution to the energy from fluctuations in the local bond order parameter. The bond order parameter is frustrated by the rotation of tangent vectors that occurs under parallel transport on a curved surface. The amount of frustration is given by the gauge field Ω_i.

To gain some physical understanding of a flexible hexatic membrane, we examine the ground states. In particular, we search for the low-temperature geometries of five- and sevenfold disclinations. After performing the minimization over θ, we find

$$\left. \frac{\delta H}{\delta \theta(\sigma)} \right|_{\theta = \theta_0} = g^{-1/2} \partial_j \left[g^{ij} (\partial_i \theta_0 - \Omega_i) \right] = 0 , \tag{2}$$

where θ_0 is the bond angle field that minimizes the energy. Upon defining

$$\partial_i \theta_0 - \Omega_i = \gamma_i{}^j \partial_j \chi , \tag{3}$$

we find that the derivative (2) is zero except when derivatives of χ do not commute. We can show that disclinations cause the derivatives to fail to commute by applying the operator $\gamma^{ki} \partial_k$ to Eq. (3) [8]:

$$\begin{aligned} D_i D^i \chi &= K - \gamma^{ki} \partial_k \partial_i \theta_0 \\ &= K(\sigma) - s(\sigma) \\ &\equiv c(\sigma) . \end{aligned} \tag{4}$$

The disclination density is given by

$$s(\sigma) = \sum_i s_i \delta(\sigma - \sigma_i) g(\sigma_i)^{-1/2} . \tag{5}$$

Here the disclination strength is given by $s_i = \pi/3$ for a fivefold disclination and $s_i = -\pi/3$ for a sevenfold disclination. Given the form of Eq. (4), we can express χ in terms of a Green's function as

$$\chi(\sigma) = \int d^2 S' G(\sigma|\sigma') c(\sigma') , \tag{6}$$

where

$$D_i D^i G(\sigma|\sigma') = \nabla_\sigma^2 G(\sigma|\sigma') = \delta(\sigma - \sigma') g(\sigma')^{-1/2} . \tag{7}$$

The Hamiltonian when the bond angle field is minimized is given by

$$\begin{aligned} H_\theta = \frac{K_A}{2} \int & d^2 S d^2 S' d^2 S'' c(\sigma') c(\sigma'') \left[\partial_i G(\sigma|\sigma') \right] g^{ij} \\ & \times \left[\partial_j G(\sigma|\sigma'') \right] . \end{aligned} \tag{8}$$

We see from Eq. (8) that the relevant quantity is not the disclination density or the Gaussian curvature separately, but rather the difference $c(\sigma)$ between them. Consequently, the hexatic energy arising from a disclination can be reduced by a nonzero Gaussian curvature. This screening, of course, will cost the membrane in terms of bending energy. The competition between screening of the hexatic energy and the bending energy determines the equilibrium shape of the membrane.

The energy of a single, isolated disclination with "charge" s in a flat, circular membrane is given by $E = (s^2/4\pi)\ln(R/a_0)$ [1]. Here R is the radius of the membrane, and a_0 is a microscopic cutoff. For five- and sevenfold disclinations, $E_5 = E_7 = (\pi K_A/36)\ln(R/a_0)$. Buckling of the membrane can reduce this energy. We describe the location of the membrane by

$$\mathbf{X}(r, \phi) = (r\sin\phi, r\cos\phi, f(r, \phi)) . \tag{9}$$

The diverging contribution to the energy comes from the large r region of the surface. The bending energy can diverge no more strongly than $\ln(R/a_0)$ in a buckled ground state, since otherwise the energy would *increase* upon buckling. This bound implies that f grows at most linearly with r. If f grows *less* rapidly than r, then the Green's function defined by Eq. (7) is given by $\partial_r G \sim 1/(2\pi r)$ as $r \to \infty$ [20]. Furthermore, the Gauss-Bonnet theorem then implies that $\int d^2 S K = 0$ for membranes with a disklike topology [21]. From Eq. (8), we see that the hexatic energy remains $E \sim (\pi K_A/36)\ln(R/a_0)$, and has not been reduced. For the logarithmic hexatic energy to be screened by buckling, therefore, the height must grow linearly with r:

$$\mathbf{X}(r, \phi) = (r\sin\phi, r\cos\phi, rh(\phi)) . \tag{10}$$

The Green's function that satisfies Eq. (7) is then given by

$$G(r, \phi) = b^{-1}\ln\left[r(1 + h(\phi)^2)^{1/2}\right] , \tag{11}$$

with

$$b = \int d\phi \frac{(1 + h^2 + h'^2)^{1/2}}{1 + h^2} . \tag{12}$$

To evaluate the hexatic Hamiltonian, we need both the Gaussian and mean curvature. For the surface defined by Eq. (9), the Gaussian curvature is proportional to a δ function

$$K(\sigma) = \alpha\delta(\sigma)g^{-1/2} . \tag{13}$$

The coefficient α can be determined from

$$\begin{aligned}
\alpha &= \int d^2 S K \\
&= \int d^2 S \gamma^{ij} \partial_i \Omega_j \\
&= \int_c d\sigma^i \Omega_i ,
\end{aligned} \tag{14}$$

where c is a contour bounding the surface. If $\mathbf{e}_1$ and $\mathbf{e}_2$ are an orthonormal basis for vectors tangent to the surface, the gauge field is given by [19]

$$\Omega_i = \mathbf{e}_1 \cdot \partial_i \mathbf{e}_2 . \tag{15}$$

From this equation we find, by taking $\mathbf{e}_1$ and $\mathbf{e}_2$ to be basis vectors in polar coordinates and subtracting the result for a flat surface,

$$\begin{aligned}
\Omega_1 &= 0, \\
\Omega_2 &= 1 - \frac{(1 + h^2 + h'^2)^{1/2}}{1 + h^2} .
\end{aligned} \tag{16}$$

We therefore conclude that

$$\alpha = 2\pi - b . \tag{17}$$

We can now perform the integrals on Eq. (8) to find

$$H_\theta = \frac{K_A(2\pi - s - b)^2}{2b}\ln(R/a_0) . \tag{18}$$

The mean curvature is given by [21]

$$\begin{aligned}
\bar{H} &= \nabla \cdot \frac{\nabla f}{(1 + |\nabla f|^2)^{1/2}} \\
&= \frac{(h + h'')(1 + h^2)}{r(1 + h^2 + h'^2)^{3/2}} .
\end{aligned} \tag{19}$$

The bending energy is then given by

$$H_\kappa = \frac{\kappa}{2}\ln(R/a_0) \int d\phi \frac{(h + h'')^2(1 + h^2)^2}{(1 + h^2 + h'^2)^{5/2}} . \tag{20}$$

The contribution to the bending energy associated with the singularity at $r = 0$ will be absorbed into a core energy. The total energy of a hexatic membrane with a single, isolated disclination, excluding the core contribution, is given by

$$\begin{aligned}
\frac{H}{\ln(R/a_0)} = {}& K_A \frac{(2\pi - s - b)^2}{2b} \\
& + \frac{\kappa}{2} \int d\phi \frac{(h + h'')^2(1 + h^2)^2}{(1 + h^2 + h'^2)^{5/2}} .
\end{aligned} \tag{21}$$

The geometry of lowest energy is found by minimizing Eq. (21) with respect to the function $h(\phi)$. Note that b depends on $h(\phi)$ through Eq. (12).

The route from the covariant Hamiltonian (1) to the tractable expression (21) is complicated. For a nearly flat surface, a simplified Hamiltonian is often used [5,8]:

$$H = \frac{K_A}{2} \int d^2 r \left[\partial_i \theta - A_i\right]^2 + \frac{\kappa}{2} \int d^2 r (\nabla^2 f)^2 , \tag{22}$$

where

$$A_i = \frac{1}{2}\epsilon_{jk}\partial_k \left[(\partial_i f)(\partial_j f)\right] , \tag{23}$$

and the derivatives are in flat space. The bond angle field $\theta_0(\sigma)$ that minimizes this energy is given by

$$\partial_i(\partial_i \theta_0 - A_i) = 0 . \tag{24}$$

To satisfy this equation, we define

$$(\partial_i \theta_0 - A_i) = \epsilon_{ij}\partial_j \chi \ . \tag{25}$$

Applying the operator $\epsilon_{ik}\partial_k$ to this equation, we find [9]

$$\nabla^2 \chi = (\partial_x^2 f)(\partial_y^2 f) - (\partial_x \partial_y f)^2 - s(\mathbf{r}) \ , \tag{26}$$

with

$$s(\mathbf{r}) = \sum_i s_i \delta(\mathbf{r} - \mathbf{r}_i) \ . \tag{27}$$

For an isolated five- or sevenfold disclination, $s(\mathbf{r}) = \pm(\pi/3)\delta(\mathbf{r})$. The Hamiltonian now reduces to

$$H = \frac{K_A}{2} \int d^2r |\nabla\chi|^2 + \frac{\kappa}{2} \int d^2r (\nabla^2 f)^2 \ . \tag{28}$$

We can further find the height function f, which minimizes this Hamiltonian. It satisfies a second, nonlinear hexatic "von Kármán equation" [9]

$$\frac{\kappa}{K_A}\nabla^4 f = (\partial_y^2 \chi)(\partial_x^2 f) + (\partial_x^2 \chi)(\partial_y^2 f)$$

$$-2(\partial_x \partial_y \chi)(\partial_x \partial_y f) \ . \tag{29}$$

With the simple Hamiltonian (22), then, we have explicit partial differential equations that define the surface of minimal energy. For the covariant Hamiltonian, the differential equation arising from minimizing Eq. (21) is much more complex.

III. THE ENERGY OF A FIVEFOLD DISCLINATION

A fivefold disclination can be screened by a surface with a positive Gaussian curvature. The natural surface to consider is a cone.

We first review the results of the approximate Hamiltonian (22). A cone defined by $f(r) = ar$ solves Eqs. (26) and (29), with $\chi(r) = -(\kappa/K_A)\ln(r/a_0)$ [9]. The coefficient is given by $a^2 = 1/3 - 2\kappa/K_A$. For $\kappa/K_A < 1/6$, the membrane buckles. The energy is given by

$$E_5 \approx \begin{cases} (\pi\kappa/3)(1 - 3\kappa/K_A)\ln(R/a_0), & \kappa/K_A < 1/6 \\ \\ (\pi K_A/36)\ln(R/a_0), & \kappa/K_A > 1/6. \end{cases} \tag{30}$$

We now review the results of the covariant Hamiltonian (1) [10]. Equation (21) fully specifies the energy, with $h = a$ and $b = 2\pi(1+a^2)^{-1/2}$. We first note that Eq. (17) can be derived from a geometrical argument. We consider capping off the cone with a small sphere of radius ϵ, as in Fig. 2. The bending energy is unaffected by this small perturbation, since we are ignoring the contribution near $r = 0$. The Gaussian curvature is zero everywhere except on the sphere. On the sphere it is given by $\alpha = \int d^2 S K = 2\pi \int_{\cos\psi}^1 du = 2\pi(1 - \cos\psi)$. With $\tan\psi = a$, we have $\alpha = 2\pi[1 - (1 + a^2)^{-1/2}]$, in agreement with Eq. (17). Upon defining $x = (1 + a^2)^{-1/2}$, we have

$$\frac{H}{\pi K_A \ln(R/a_0)} = \frac{(1/6 - 1 + x)^2}{x} + \frac{\kappa}{K_A}\frac{1 - x^2}{x} \ . \tag{31}$$

Minimization of this equation leads to

$$E_5 = \begin{cases} \pi K_A \left\{ 2\left[(25/36 + \kappa/K_A)(1 - \kappa/K_A)\right]^{1/2} - 5/3 \right\} \\ \qquad \times \ln(R/a_0), \quad \kappa/K_A < 11/72 \\ \\ (\pi K_A/36)\ln(R/a_0), \quad \kappa/K_A > 11/72. \end{cases} \tag{32}$$

We note that the limit $K_A \rightarrow \infty$ corresponds to the inextensional limit of a crystalline membrane. This energy has the correct limit $E_5 \rightarrow (11\pi\kappa/30)\ln(R/a_0)$ as $K_A \rightarrow \infty$, which corresponds to a *crystalline* membrane [6]. While the Hamiltonian (22) is often thought of as valid for small ∇f, we see that it does not exactly predict the buckling transition, where ∇f is indeed a small, nonzero constant.

When $\kappa/K_A > 11/72$, the above calculation shows that the height grows sublinearly with r. In fact, we now show that the height grows with a power that depends continuously on κ/K_A. We assume that $f(r,\phi) = f(r)$. The hexatic and bending energies of Eq. (1) are then given by

$$F_\theta = \pi K_A \int_1^\infty dr \frac{(1 + f'^2)^{1/2}}{r} \left[\frac{1}{(1 + f'^2)^{1/2}} - \frac{5}{6}\right]^2 ,$$

$$F_\kappa = \pi\kappa \int_1^\infty dr \frac{(1 + f'^2)^{1/2}}{r}$$

$$\times \left[\frac{f'}{(1 + f'^2)^{1/2}} + \frac{rf''}{(1 + f'^2)^{3/2}}\right]^2 \ . \tag{33}$$

We have set the short-range cutoff to $a_0 = 1$. As we shall see, $f' \rightarrow 0$ as $r \rightarrow \infty$, when $\kappa/K_A > 11/72$. Upon expanding Eq. (33) for small f', we find

$$F \sim \pi \int_1^\infty dr \left[\frac{K_A}{36r} + \frac{\kappa(f' + rf'')^2}{r} - \frac{11K_A f'^2}{72r}\right]$$

$$+O(f^4) \ . \tag{34}$$

Upon solving the equation $\delta F/\delta f(r) = 0$, we find in the case of constant moduli

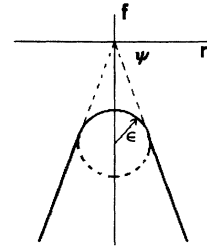$$f(r) \sim ar^{1-y} \quad \text{as} \quad r \rightarrow \infty \ , \tag{35}$$

FIG. 2. Cone $f(r) = ar$, shown in projection, capped by a small sphere used to calculate the integrated Gaussian curvature. The angle ψ is given by $\tan\psi = a$.
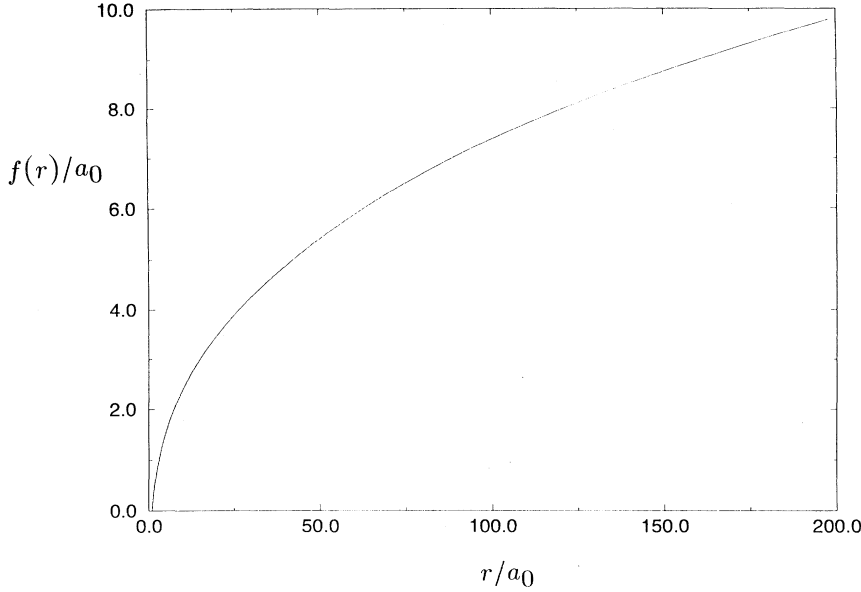
FIG. 3. Height of an "unbuckled" membrane with a fivefold disclination as a function of r for the case $\kappa/K_A = 1/4$. There is a short distance cutoff so that $f(r)$ is undefined for $r < a_0$.

with

$$y = [1 - 11K_A/(72\kappa)]^{1/2} . \tag{36}$$

We also minimize Eq. (33) numerically. We express $f'(r)$ on a grid at grid points $r_i = \exp(\ln r_{\max} i/n)$ and approximate the integral by a sum and derivatives by finite difference. We found convergence was achieved for $n = 200, r_{\max} = 100$. Results are presented for $n = 400, r_{\max} = 200$. The Polak-Ribiere conjugate gradient method was used to determine $f'(r_i)$ [22]. Figure 3 shows the height as a function of r for the specific case $\kappa/K_A = 1/4$. The numerical results reproduce the asymptotic scaling of Eq. (35). The energy of this ground state is $E_5 = (\pi K_A/36)\ln R - 0.0281\pi K_A + E_c$, where E_c is a core energy contribution. If this core contribution is sufficiently large in the deformed state, the surface of minimal energy may be flat, and the constant a in Eq. (35) can be zero.

IV. THE ENERGY OF A SEVENFOLD DISCLINATION

A sevenfold disclination can be screened by a surface with a negative Gaussian curvature. There is no obvious natural surface to consider in this case. Using the approximate Hamiltonian (22), we can achieve an analytical answer, however. We let

$$f(r, \phi) = ar\sin 2\phi,$$
$$\chi(r) = \frac{3\kappa}{K_A}\ln(r/a_0) . \tag{37}$$

Equation (29) is solved by this choice. Equation (26) is solved provided that $a^2 = 2/9 - 4\kappa/K_A$. When $\kappa/K_A < 1/18$, the membrane buckles. The energy is given by

$$E_7 \approx \begin{cases} (\pi\kappa)(1 - 9\kappa/K_A)\ln(R/a_0), & \kappa/K_A < 1/18 \\ \\ (\pi K_A/36)\ln(R/a_0), & \kappa/K_A > 1/18. \end{cases} \tag{38}$$

The covariant Hamiltonian (1) does not yield so easily to an analytical treatment. We can, however, expand Eq. (21) for small h to find the buckling transition:

$$\frac{\delta H}{\delta h(\phi)} = 0 = \frac{13K_A}{72}(h + h'')$$
$$+ \kappa(h + 2h'' + h'''') + O(h^3) . \tag{39}$$

This equation predicts buckling for $\kappa/K_A < 13/216$ with $h(\phi) = a\sin 2\phi$. Again the approximate Hamiltonian (22) predicts the transition value only approximately.

We determine the surface that minimizes the energy for general values of κ/K_A by numerically identifying the function $h(\phi)$ that minimizes Eq. (21). We express $h(\phi)$ on a grid at grid points $\phi_i = 2\pi i/n$, again approximating the integral by a sum and derivatives by finite difference. We found that convergence was achieved for $n = 100$. Results are presented for $n = 200$. The Polak-Ribiere conjugate gradient method was used to determine the $h(\phi_i)$ [22].

Figure 4 presents the numerically determined energies H_θ, H_κ, and H. The membrane buckles when $\kappa/K_A < 0.060$, in good agreement with the exact value of 13/216. As the membrane becomes less stiff, the buckling is able to screen more and more of the hexatic energy: the hexatic energy goes from

$$H_\theta \sim (\pi K_A/36)\ln(R/a_0) \quad \text{for} \quad \kappa/K_A \geq 13/216 \tag{40}$$

to

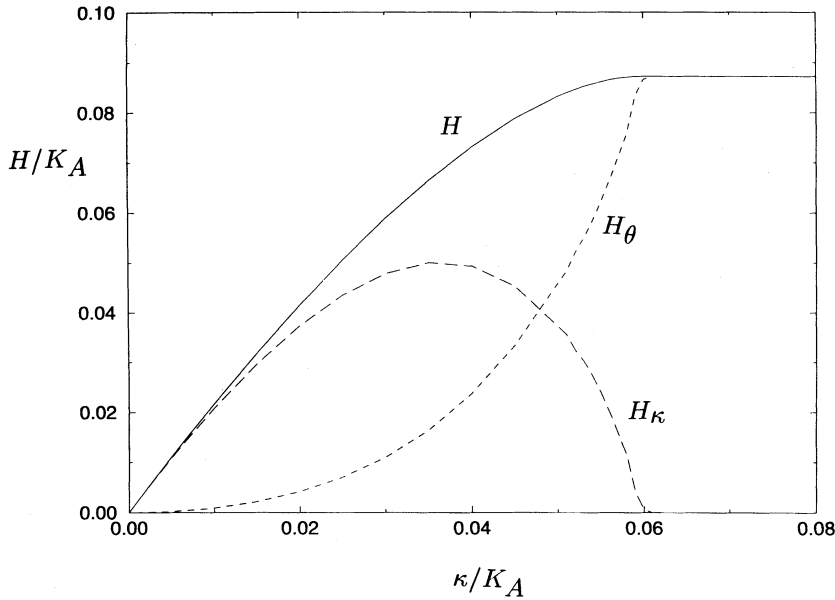$$H_\theta \sim 0 \quad \text{as} \quad \kappa/K_A \to 0, \tag{41}$$

FIG. 4. Hexatic (short-dashed curve), bending (long-dashed curve), and total (solid curve) energies when $r \to \infty$ as a function of κ/K_A for a sevenfold disclination. An overall factor of $\ln(R/a_0)$ has been suppressed in each term. The defect is unbuckled for $\kappa/K_A > 13/216 \approx 0.060$.

as expected. Similarly, the bending energy goes from

$$H_\kappa \sim 0 \quad \text{for} \quad \kappa/K_A \geq 13/216 \tag{42}$$

to

$$H_\kappa \sim 2.27\kappa \ln(R/a_0) \quad \text{as} \quad \kappa/K_A \to 0 . \tag{43}$$

The limit as $\kappa/K_A \to 0$ agrees with numerical calculations for inextensional crystalline membranes [6].

Figure 5 shows the function $h(\phi)$ for various values of the ratio κ/K_A. As expected, the surface is flatter for stiffer surfaces. For very flexible membranes, the surface converges to a limiting shape. This limiting shape is very nearly proportional to $\sin 2\phi$, as shown in Fig. 6. More

generally, we can expand $f(r, \phi)$ in a Fourier series

$$f(r, \phi) \sum_{m=0}^{\infty} f_m(r) \cos(m\phi) , \tag{44}$$

where $f_m(0) = 0$. All odd terms must vanish for a twofold symmetric saddle point configuration. In addition, f should change sign under a $\pi/2$ rotation, which eliminates the terms in Eq. (44) with $m = 0, 4, 8, \ldots$. Such a symmetric saddle has an expansion of the form

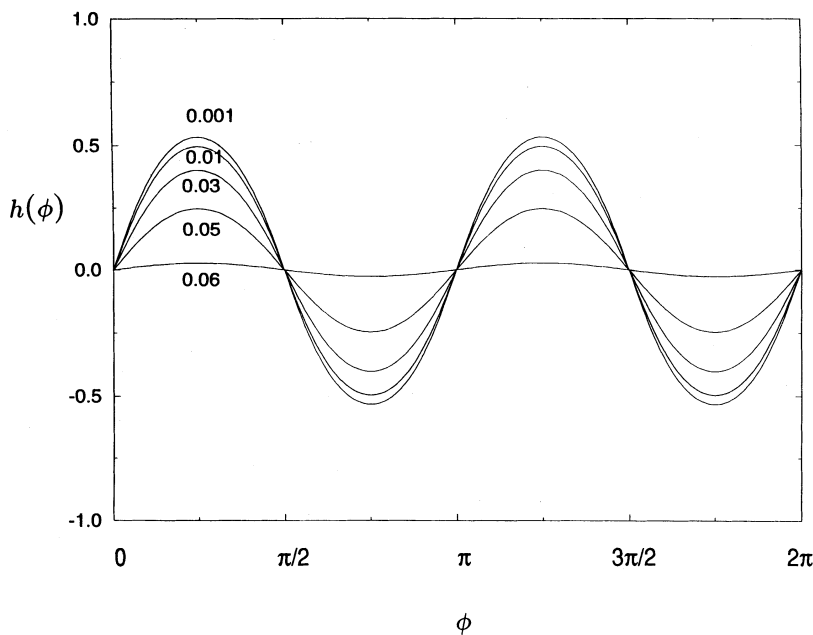$$f(r, \phi) \sum_{p=0}^{\infty} f_{4p+2}(r) \cos\left[2(2p+1)\phi\right] , \tag{45}$$

FIG. 5. Surface $h(\phi)$ for a sevenfold defect above its unbuckling transition for the cases $\kappa/K_A = 0.06, 0.05, 0.03, 0.01,$ and 0.001.
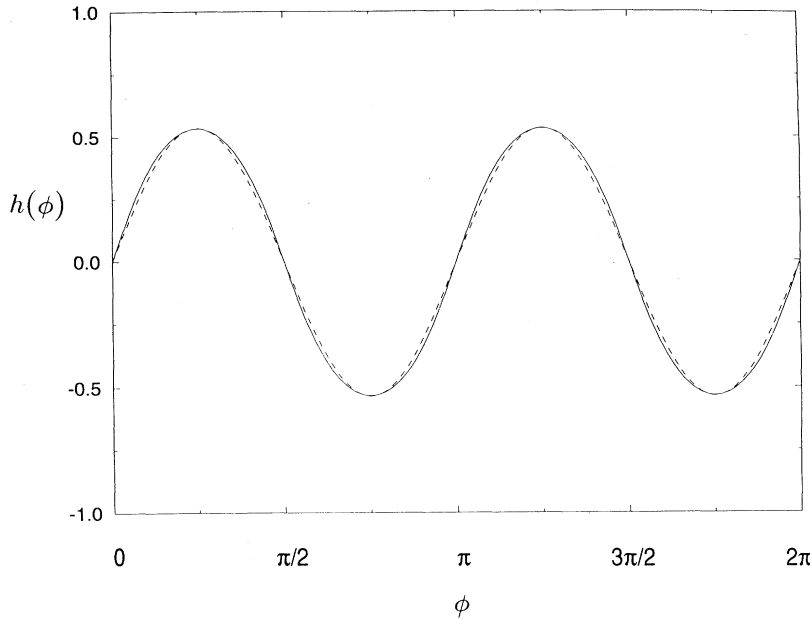
FIG. 6. Surface $h(\phi)$ in the limit $\kappa/K_A \to 0$ (solid curve), which mimics the behavior in a crystalline solid, and the function $0.534\sin(2\phi)$ (dashed curve) for a sevenfold defect.

a conclusion also reached by Park and Lubensky [14]. We have checked numerically that the only nonzero Fourier components in Eq. (44) are indeed of the form $m = 4p+2$, although the $m = 2$ term alone provides an excellent approximation.

When $\kappa/K_A > 13/216$, the height grows sublinearly with r. Just as for the fivefold disclination, the height grows with a power that depends continuously on κ/K_A. To see this, note first that when $\kappa/K_A > 13/216$, $\nabla f \to 0$ as $r \to \infty$. Upon expanding Eq. (1) for small ∇f, we find

$$
F \sim \frac{K_A}{144} \int dr d\phi \ \{2/r + 13(\partial_r f)^2/r + 11(\partial_\phi f)^2/r^3
$$
$$
-12[\partial r(\partial_\phi f)^2]/r^2\}
$$
$$
+ \frac{\kappa}{2} \int dr d\phi \ r \left[\partial_r^2 f + (\partial_r f)/r + (\partial_\phi^2 f)/r^2\right]^2
$$
$$
+ O(f^4) \ .
\tag{46}
$$

The solution of $\delta F/\delta f(r,\phi) = 0$ is

$$
f(r) \sim a r^{1-y} \sin 2\phi \quad \text{as} \quad r \to \infty \ ,
\tag{47}
$$

with

$$
y = [720 + 13K_A/\kappa - (331\,776 + 29\,952 K_A/\kappa
$$
$$
+169 K_A^2/\kappa^2)^{1/2}]^{1/2}]/12 \ .
\tag{48}
$$

As in the case of fivefold disclinations, this sublinear decay leads to an additive, constant correction to the logarithmically diverging energy as $R \to \infty$.

V. THERMAL FLUCTUATIONS

We have so far ignored thermal fluctuations of the hexatic membrane. This assumption is valid only for the $T \to 0$ limit. For finite temperatures and for large mem-

branes, thermal fluctuations will become important.

A complete discussion of thermal effects is beyond the scope of this paper. We can, however, use the results of David et al. [12] and of Park and Lubensky [13] to estimate how the structure of disclinations in hexatic membranes is modified at finite temperatures. Park and Lubensky argue that proper implementation of an ultraviolet cutoff to fluctuations in hexatic membranes leads to the replacement

$$
K_A \to K_A^{\mathrm{eff}} = K_A - \frac{3}{32\pi} k_B T (K_A/\kappa)^2 \ .
\tag{49}
$$

The bending rigidity κ is unchanged. In the absence of a nonzero disclination density, the remaining renormalization equations for κ and K_A^{eff} are those found originally by David et al. [12]:

$$
\frac{dK_A^{\mathrm{eff}}}{dl} = 0,
$$
$$
\frac{d\kappa/k_B T}{dl} = -\frac{3}{4\pi}\left(1 - \frac{K_A^{\mathrm{eff}}}{4\kappa}\right) \ .
\tag{50}
$$

The renormalization group flows induced by these equations are indicated schematically by the arrows in Fig. 1.

We apply these results to the dilute limit of isolated disclinations discussed in Secs. IV and V. The locus of disclination unbinding transitions, given by the criteria $F_5(\kappa, K_A) \equiv 0$ and $F_7(\kappa, K_A) \equiv 0$ discussed in the Introduction, is shown as the solid and dashed lines in Fig. 1. When thermal fluctuations are superimposed on the solutions of the $T = 0$ extremal equations for disclinations in a membrane of size R, standard finite size scaling arguments suggest that the couplings controlling the defect energies on this scale should be the *running* coupling constants $K_A^{\mathrm{eff}}(l)$ and $\kappa(l)$ obtained from Eq. (50) evaluated at $l = \ln(R/a_0)$. Effects of thermally excited

bound disclination pairs on an otherwise isolated defect could be included by adding a vortex fugacity to the set of recursion relations [13]. We then expect that Eqs. (33) and (46) should be replaced by expressions where K_A and κ are replaced by the functions $K_A^{\rm eff}(l = \ln r/a_0)$ and $\kappa(l = \ln r/a_0)$ appearing inside the integrals over r. Although $K_A^{\rm eff}$ does not renormalize at this order, a non-trivial renormalization could appear when higher-order corrections in $k_B T/\kappa$ and $k_B T/K_A^{\rm eff}$ are included.

If the basin of attraction of the locally stable fixed line in Fig. 1 includes the entire hexatic phase, $K_A^{\rm eff}(r)$ and $\kappa(r)$ will always be driven as $r \to \infty$ into the unbuckled regime for both five- and sevenfold disclinations, since $\lim_{r\to\infty} \kappa(r)/K_A^{\rm eff}(r) = 1/4$. The bending energy will then not contribute to the logarithmically diverging part of the energy, and both defects should unbind

at the same point. Although "unbuckled" in this sense, the limited disclination shapes will be characterized by the power laws (35) and (47), with $\kappa/K_A = 1/4$. For fivefold defects we find the asymptotic shape is given by $y = y_+ = 0.6236$, while for sevenfold defects we have $y = y_- = 0.8249$.

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