Kosterlitz-Thouless Transitions on Fluctuating Surfaces

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Abstract

We investigate the Kosterlitz-Thouless transition for hexatic order on a free fluctuating membrane and derive both a Coulomb gas and a sine-Gordon Hamiltonian to describe it. In the former, both disclinations and Gaussian curvature contribute to the charge density. In the latter, there is a linear coupling between a scalar field and the Gaussian curvature. We derive renormalization group recursion relations that predict a transition with decreasing bending rigidity $\kappa$. Using the sine-Gordon model, we show that there is no KT transition on a deformable sphere.

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A fluid membrane can be modeled as an ideal fluctuating surface whose energy depends only on its geometry. If the membrane is free from external tension, the dominant term in this energy is the Helfrich-Canham bending energy [1,2] with bending rigidity $\kappa$. Such a membrane with a molecular length $a$ is crumpled at length scales beyond the persistence length, $\xi_p = ae^{4\pi\kappa/3T}$, at which the renormalized bending rigidity passes through zero [3]. Membranes with hexatic tangent plane orientational order are stiffer than fluid membranes [4]. A flat membrane has quasi-long-range (QLR) hexatic order at low temperature and undergoes a Kosterlitz-Thouless (KT) disclination unbinding transition to a disordered state [5]. A free hexatic membrane at low temperature exists in a “crinkled” state with QLR hexatic order and a nonzero long-wavelength bending rigidity [7,8].

Free hexatic membranes are predicted [8] to undergo a KT transition from the crinkled phase to the crumpled fluid phase. To our knowledge, however, there has been no systematic treatment of this transition with complete renormalization group recursion relations for the hexatic stiffness $K$ and disclination fugacity $y$ associated with the KT transition in addition to the bending rigidity $\kappa$ controlling membrane height fluctuations. In this paper, we present an analysis of the KT transition on a fluctuating membrane using both the Coulomb gas model obtained directly from the hexatic Hamiltonian and the sine-Gordon model dual to the Coulomb gas model. A more detailed presentation will appear in a separate publication.

Both local Gaussian curvature and disclinations contribute to the charge density of the coulomb gas. The bare hexatic rigidity $K$ plays the role of the square of one of the charges in the Coulomb gas. The other charge is determined by $K$ and the Liouville action [7]. As in electrodynamics, neither charge undergoes a renormalization in agreement with Ref. [7], which found that $K$ did not renormalize. We find, however, that fluctuations in Gaussian curvature reduce the dielectric constant even in the absence of disclinations and lead to a decrease with decreasing $\kappa$ of the effective hexatic rigidity that controls correlations of the hexatic order parameter. As a result, we find, in contrast to previous treatments [4,8] that decreasing $\kappa$ leads to a KT transition from the crinkled to the crumpled state as depicted in Fig. [1]. We obtain recursion relations for $K$, $y$, and $\kappa$ that yield a KT transition and


that allow us to calculate quantities such as the persistence length in the crumpled phase. We find that \( \xi_p \sim \xi_{KT} e^{4\pi \kappa/3T} \) where \( \xi_{KT} \sim a \exp(\pi/b\sqrt{T - T_c}) \) is the KT correlation length when \( \kappa \) is large and the persistence length is larger than the \( \xi_{KT} \).

The sine-Gordon model we derive applies to an open membrane and to closed membranes (vesicles) of arbitrary genus \( h \). As on flat surfaces, this model has a scalar field \( \phi \) with a gradient and a \( \cos \phi \) energy. The principal coupling to geometry occurs via an interaction, similar to the dilaton coupling of string theory [9], proportional to \( \phi R \) with an imaginary coefficient, where \( R \) is the scalar or intrinsic curvature. Using standard renormalization group techniques for the sine-Gordon model [10], we obtain the same recursion relations as we obtain using the Coulomb gas. We further show that shape fluctuations on a sphere, like gauge fluctuations in an infinite two-dimensional superconductor, generate a “mass” for \( \phi \) and depress the KT transition temperature to absolute zero.

Membrane coordinates in three space are specified by a vector \( \mathbf{R}(\tilde{u}) \) as a function of a two-dimensional parameter \( \tilde{u} = (u^1, u^2) \). The metric tensor \( g_{ab} = \partial_a \mathbf{R}(\tilde{u}) \cdot \partial_b \mathbf{R}(\tilde{u}) \), its inverse \( g^{ab} \), and the curvature tensor \( K_{ab} = \mathbf{N} \cdot \partial_a \partial_b \mathbf{R} \), where \( \partial_a = \partial/\partial u^a \) and \( \mathbf{N} \) is the unit normal to the surface, can be constructed from \( \mathbf{R} \). The energy of a free membrane is described by the Helfrich-Canham Hamiltonian [1]

\[
\mathcal{H}_\kappa = \frac{1}{2} \kappa \int d^2u \sqrt{g} H^2,
\]

where \( g = \det g_{ab} \) and \( H = g^{ab} K_{ab} \) is twice the mean or extrinsic curvature. A membrane with hexatic order has an order parameter \( \psi = |\psi| e^{6i\theta} \). A membrane with generalized \( p \)-atic order has an order parameter \( \psi = |\psi| e^{ip\theta} \) invariant under \( \theta \rightarrow \theta + (2\pi/p) \). The elastic energy associated with spatial variations of \( \theta \) for system with \( p \)-atic order is [5]

\[
\mathcal{H}_\theta = \frac{1}{2} K \int d^2u \sqrt{g} g^{ab} (\partial_a \theta - A_a)(\partial_b \theta - A_b),
\]

where \( A_a \) is the spin connection satisfying \( \gamma^{ab} \partial_a A_b = S \), where \( \gamma^{ab} \) is the antisymmetric tensor with magnitude \( g^{-1/2} \), and \( S = \det K_a^b = R/2 \) is the Gaussian curvature. The total long wavelength Hamiltonian for a \( p \)-atic membrane is then \( \mathcal{H} = \mathcal{H}_\kappa + \mathcal{H}_\theta \). In the presence
of disclinations, which have strength $q = k/p$ where $k$ is an integer, $\partial_a \theta$ becomes singular: $\partial_a \theta = \partial_a \tilde{\theta} + v_a$. The singular part satisfies $\gamma^{ab} \partial_a v_b = n$, where $n = 2\pi g^{-1/2} \sum_{\alpha} q_{\alpha} \delta(\bar{u} - \bar{u}_{\alpha})$ is the disclination density arising from disclinations of strength $q_{\alpha}$ at positions $\bar{u}_{\alpha}$. Thus $-\Delta_g (v_a - A_a) = \gamma^a_b \partial_b (n - S)$, where $\Delta_g = D_a D^a$ is the covariant Laplacian operator on a surface with metric tensor $g_{ab}$. Using this relation, $\mathcal{H}_\theta$ can be expressed as the sum of a regular part depending only on $\tilde{\theta}$ and a curved space generalization of the energy of a 2D Coulomb gas: $\mathcal{H}_\theta = \mathcal{H}_{\text{reg}} + \mathcal{H}_c$ with

$$\mathcal{H}_{\text{reg}} = \frac{1}{2} K \int d^2 u \sqrt{g^{ab}} \partial_a \tilde{\theta} \partial_b \tilde{\theta},$$

$$\mathcal{H}_c = \frac{1}{2} K \int d^2 u \sqrt{|\rho|} (-\Delta_g)^{-1} \rho,$$

where $\rho = n - S$ is the total “charge density” arising from disclinations and Gaussian curvature. Then, using $\int \mathcal{D} \tilde{\theta} e^{-\beta \mathcal{H}_{\text{reg}}} = e^{-\beta \mathcal{H}_L}$ where $\beta \mathcal{H}_L = -S_L/(96 \pi)$ and $S_L$ is the Liouville action \[11\]

$$S_L = \int d^2 u \sqrt{|R|} (-\Delta_g)^{-1} R,$$

we can write the partition function as

$$Z(\kappa, K, y) = \text{Tr}_v \int \mathcal{D} \mathcal{R} \mathcal{D} \tilde{\theta} y^N e^{-\beta \mathcal{H}_\kappa - \beta \mathcal{H}_\theta}$$

$$= \text{Tr}_v \int \mathcal{D} \mathcal{R} e^{-\beta \mathcal{H}_\kappa - \beta \mathcal{H}_L - \beta \mathcal{H}_c} y^N.$$

Here $\mathcal{H}_\theta$ and $\mathcal{H}_c$ are understood to depend on the total number of vortices $N$ and on the position and charge of each vortex, $\text{Tr}_v$ is the trace over vortices with appropriate factors of $N!$, and $\mathcal{D} \mathcal{R}$ is the measure for fluid membranes, which includes the Fadeev-Popov determinant and Liouville factor \[12\]. If we include only the lowest strength vortices with $q_{\alpha} = \pm 1/p$, then $\text{Tr}_v$ can be defined via

$$\text{Tr}_v = \sum_{N_+, N_-} \delta_{N_+ - N_- - p \chi} \frac{1}{N_+! N_-!} \int [\mathcal{D} u^+]_{N_+} [\mathcal{D} u^-]_{N_-},$$

where $N_\pm$ is the number of disclinations with strength $\pm 1/p$, $\chi = 2(1 - h)$ is the Euler characteristic of the surface, and $[\mathcal{D} u^\pm]_{N_\pm} = \prod_{\alpha}^{N_\pm} d^2 u_\alpha [g(u_\alpha^\pm)]^{1/2} / a^2$ is the integration measure.
for the positions of the $N_\pm$ charges with sign $\pm$. The Kroneker $\delta$ imposes the constraint that the total disclination strength equal the Euler characteristic $\chi$. On an open surface, the long-range Coulomb potential leads to $N_+ = N_-$, and we can use $\text{Tr}_\nu$ with $\chi = 0$. We can convert the Coulomb gas model \[\text{Eq. (6)}\] to a sine-Gordon model by representing the factor $e^{-\beta H_c}$, via a Hubbard-Stratonovich transformation, as

$$e^{-\beta H_c} = e^{\beta H_L} \int D\phi e^{-\int d^2u \sqrt{g} \left( \frac{1}{2} \partial_\alpha \phi \partial^\alpha \phi - \frac{1}{2} \gamma \int d^2u \sqrt{g} \cos \phi - i \lambda \int d^2u S \right)},$$

where the factor $e^{\beta H_L}$ assures that $e^{-\beta H_c}$ is one when $\rho = 0$. Then, setting $\delta_{N,0} = (1/2\pi) \int_0^{2\pi} d\omega e^{-i\omega N}$, integrating over $[Du^+]_{N_+}[Du^-]_{N_-}$, and shifting $\phi \rightarrow p\phi/(2\pi) - \omega$, we obtain

$$Z = \int DRD\phi e^{-\mathcal{L}},$$

where

$$\mathcal{L} = \beta H_k + \frac{1}{2} \gamma \int d^2u \sqrt{g} \partial_\alpha \phi \partial^\alpha \phi - \frac{2y}{a^2} \int d^2u \sqrt{g} \cos \phi - i \lambda \int d^2u S,$$

(7)

where $\gamma = p^2/(4\pi^2\kappa)$ and $\lambda = p/(2\pi)$. This effective action is valid for a surface of arbitrary genus. The coupling between $\phi$ and geometry is via a $\phi S$ term analogous to the dilaton coupling of string theory \[\text{[9]}\].

Eqs. (5), (6), and (7) provide us with three equivalent versions of the partition function for $p$-atic order on a fluctuating membrane, all of which can be used to study the KT crinkled-to-crumpled phase transition. We focus first on the Coulomb gas model on a nearly flat surface. The Monge gauge with $\tilde{u} = x = (x, y)$ and $R(x) = (x, h(x))$ provides the most natural description of such a surface. In this gauge, the Gaussian curvature is $S = -\frac{1}{2} \left( \partial^2 \delta_{ij} - \partial_i \partial_j \right) h \partial_i \partial_j h$ to lowest order in $h$. Interactions among charges in a Coulomb gas are screened by other charges. In our Coulomb gas, there are two kinds of charges: disclination charge and Gaussian curvature charge. We are interested in the charge density $\rho = n - S$. The dielectric constant associated with this charge density is

$$\epsilon^{-1}(q) = 1 - (\beta K/q^2) C_{pp}(q),$$

(8)

where

$$C_{pp}(q) = \int d^2x e^{-i\mathbf{q} \cdot (\mathbf{x} - \mathbf{x}')} \langle \sqrt{g(x)} \rho(x) \sqrt{g(x')} \rho(x') \rangle,$$

5
is the charge density correlation function. This expression for $\epsilon^{-1}$ is identical to the corresponding flat space expression except that $\sqrt{g}\rho$ replaces $\rho$ in $C_{\rho\rho}$. The effective or renormalized stiffness $K_R$ is related in the usual way to the zero $q$ limit of $\epsilon^{-1}$: $\beta K_R = \lim_{q \to 0} \beta K \epsilon^{-1}$. $C_{\rho\rho}(q)$ is the complete $\rho - \rho$ correlation function. It depends on all interactions in Eq. (6), including the Liouville term $\beta \mathcal{H}_L$. We are interested in situations in which the disclination density, or equivalently $y$, is small, and we consider first the case $y = 0$ for which there is only Gaussian curvature charge. Then $C_{\rho\rho}(q) = C^0_{SS}(q)$, and $\beta \mathcal{H}_L + \beta \mathcal{H}_c$ is equal to $\beta \mathcal{H}_c(S = 0)$ with $K$ replaced by $\beta K' = \beta K - (12\pi)^{-1}$ in agreement with Ref. [7].

The correlation function $C^0_{SS}(q)$ can be expressed in terms of a polarization bubble $P(q)$ as $\beta \mathcal{K} = \lim_{q \to 0} \beta K \epsilon^{-1}$. Thus, in the absence of disclinations, the renormalized rigidity is $\beta K' = \beta K - (3/32\pi)(K/\kappa)^2$. It is straightforward to verify that the correlation $g(x) = \langle \cos(\theta(x) - \theta(0) - \int_0^x ds_a A^a) \rangle$ between a spin at the origin and a spin at $x$ parallel transported to the origin decays with $|x|$ with an exponent determined by $K_R$ rather than $K$: $g(x) \sim |x|^{-2\pi\beta K}$, which reduces when $y = 0$ to $|x|^{-2\pi\beta K}$.

Next we consider the order $y^2$ terms arising from disclinations. To lowest order in $\beta \kappa$, the disclination density correlation function $C_{nn}(q)$ has the same form as it has in flat space:

$$C^0_{nn}(q) = q^2 4\pi^3 y^2 \int_a^\infty dr r^{3 - 2\pi\beta K},$$

where $a$ is the short distance cutoff. The cross correlation function $C_{ns}(q)$ is also of order $y^2$ and equal to $\beta K C^0_{SS}(q) C^0_{nn}(q)/q^2$. An expansion in powers of $\beta K/\beta \kappa$ then yields

$$C^0_{nn}(q) = q^2 4\pi^3 y^2 \int_a^\infty dr r^{3 - 2\pi\beta K}.$$

This is identical to the equation for $K_R$ on a rigid flat surface but with $\beta \mathcal{K}^{-1} = (\beta K) - (3/32\pi)(\beta \kappa)^{-2}$ replacing $(\beta K)^{-1}$. It yields the KT recursion relations for $\beta \mathcal{K}$ and $y$. To these we must add the equation governing the renormalization of $\kappa$. To lowest order in the temperature $\beta^{-1}$ and $y^2$, the equation governing $\kappa$ is identical to that derived in Ref.
To leading order in $\beta^{-1}$ and $y$, we can replace $K$ by $\overline{K}(l)$ in the equation for $\kappa$. Our recursion relations to lowest order in $\beta^{-1}$ and $y$ are

\begin{align}
\frac{d(\beta K)^{-1}}{dl} &= \frac{4\pi^2}{p^2} y^2 \\
\frac{dy}{dl} &= \left(2 - \frac{\pi \beta K}{p^2}\right)y \\
\frac{d\beta \kappa}{dl} &= -\frac{3}{4\pi} \left(1 - \frac{\beta \overline{K}}{4\beta \kappa}\right).
\end{align}

We have also derived these equations directly from the sine-Gordon model using the procedure or Ref. [10]. They are what one would have expected. The first two equations are exactly the KT equations, but with $\beta K$ replaced by $\beta \overline{K}$. Similarly, the equation controlling $\beta \kappa$ is identical to that derived using a momentum shell renormalization procedure in Refs. [4] but again with $\beta \overline{K}$ replacing $\beta K$. Eqs. (11) to (13) have a fixed line corresponding to the crinkled phase at $y = 0$, $\beta \kappa = \beta \overline{K}/4$ independent of $p$. At $\beta \overline{K} = \beta \overline{K}^* = 2/\pi$, the system becomes unstable with respect to the formation of disclinations, and there is a KT transition to a fluid phase with unbound disclinations. For $(\beta \overline{K})^{-1} > (\beta \overline{K}^*)^{-1}$, $\beta \overline{K}$ decreases with $l$, and the ratio $\beta \overline{K}/\beta \kappa$ tends to zero so that Eq. (13) for $\beta \kappa$ tends to that for a free fluid membrane. An alternative route to the derivation of Eqs. (11) and (12) is to integrate out height fluctuations to produce an effective theory for $\theta$ (or $\phi$ in the sine-Gordon model) on a coarse-grained flat surface. This effective theory is identical to the usual flat space theory with $\overline{K}$ replacing $K$.

In the vicinity of the KT critical point, $y = 0$, $\beta \overline{K} = \beta \overline{K}^*$, $\beta \kappa = \beta \kappa^* \equiv \beta \overline{K}^* / 4$, we can set $\beta \overline{K} = \beta \overline{K}^*(1 - x)$, and $\beta \kappa = \beta \kappa^*(1 - z)$. To lowest nontrivial order in $x, y, z$, Eqs. (11) to (13) become

\begin{align}
\frac{dx}{dl} &= 8\pi^2 y^2, \quad \frac{dy}{dl} = 2xy \\
\frac{dz}{dl} &= \frac{3}{2} \left[x - (1 - x)z\right].
\end{align}

The flow lines for these equations are shown in Figs. 1 and 3. In the $xy$ plane (Fig. 2c), flows are identical to the KT flows. In the $xz$ plane (Fig. 2a), there is some curvature in the
flows toward the fixed line resulting from couplings to $y$. In addition, flows are away from the critical line $x = 0$. Neither of these effects was observed in previous treatments ignoring $y$. Fig. 1b shows flows in the $(\beta K)^{-1} - (\beta \kappa)^{-1}$ rather than the $(\beta K)^{-1} - (\beta \kappa)^{-1} $ plane. This shows that the crinkled phase exists only in a region near the origin with both $(\beta K)^{-1}$ and $(\beta \kappa)^{-1}$ small. Thus, decreasing the bending rigidity $\kappa$ will lead to disordering to the fluid phase. This effect is not apparent in the treatment of Ref. [8].

The persistence length in the fluid phase can be obtained with the aid of Eqs. (14) to (15). $\beta K$ reaches 0 when $x = 1$, and does not become negative. We may, therefore, use Eq. (14) to determine $x(l)$ for $l < l_0$ where $x(l_0) = 1$. The KT correlation length is

$$\xi_{KT} = a e^{l_0} = a \exp[\pi/\sqrt{b(T - T_c)}].$$

For $l > l_0$, we set $x(l) = 1$. Thus $z(l)$ satisfies Eq. (15) for $l < l_0$ and $dz/dl = 3/2$ for $l > l_0$, and

$$z(l) = \begin{cases} z_0 + F(l), & \text{if } l \leq l_0 \\
2z_0(l - l_0) + F(l_0) & \text{if } l > l_0, \end{cases}$$

(16)

where $z_0 = 1 - (\beta \kappa/\beta \kappa^*)$ and $F(l) = \int_0^l dl e^{-\psi(l)} x(l)$ with $\psi(l) = (3/2) l_0^2 \int_0^l dl (1 - x(l))$. The persistence length is then $\xi_p = a e^{l_*}$ where $z(l_*) = 1$. For large $\kappa$, $l_* > l_0$, and $\xi_p = a e^{F(l_0)} \xi_{KT} e^{4\pi \kappa/3T}$. For smaller $\kappa$ and for $\beta K$ near the critical point, $l_*$ may be less than $l_0$ and $\xi_p$ can be less than $\xi_{KT}$.

The sine-Gordon model of Eq. (7) applies to surfaces of arbitrary genus. It can be used to investigate the effect of nonzero Gaussian curvature on the KT transition. On a nearly spherical surface of genus zero, we can parametrize the surface by its radius vector as a function of solid angle $\Omega$: $R(\Omega) = R_0(1 + \eta(\Omega)) e_r$, where $e_r$ is the unit radius vector. To lowest order in $\eta$,

$$\mathcal{L} = -\frac{1}{2} \beta \kappa \int d\Omega ((\nabla^2 + 2) \eta)^2 + \frac{1}{2} \gamma \int d\Omega (\nabla \phi)^2$$

$$- i \lambda \int d\Omega \phi (\nabla^2 + 2) \eta + \frac{2y}{(a/R_0)^2} \int d\Omega \cos \phi,$$

(17)

where $\nabla$ is the gradient on a spherical surface of unit radius. Note that there is a linear coupling between $\phi$ and $\eta$. In the case of a nearly flat membrane, this coupling was proportional to $\phi(\nabla^2 h)^2$ and thus of higher order in normal displacements of the surface. An
effective theory on the reference spherical surface can be obtained by integrating out the height fluctuations. The resulting action is

\[
\mathcal{L} = \frac{1}{2} \gamma \int d\Omega \phi [-\nabla^2 + (K/\kappa)] \phi + \frac{2y}{(a/R_0)^2} \int d\Omega \cos \phi.
\]

The important feature of this model is the “mass term”, \((K/\kappa)\phi^2\) that suppresses fluctuations in \(\phi\) and keeps the system in the ordered phase of the sine-Gordon model or, alternatively, in the disordered phase of the Coulomb gas model. If \(K/\kappa > 1\), the transition is suppressed altogether, much as the KT transition is suppressed in an infinite 2D superconductor. If on the other hand \(K/\kappa \ll 1\), there can be an effective transition. In particular, when \(\kappa \to \infty\), the KT transition on a rigid sphere is regained.

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FIG. 1. Renormalization flows obtained from Eqs. (14) and (15) in (a) the \((x, z)\) or \((\beta K, \beta \kappa)\)-plane and (b) in the \((\beta K, \beta \kappa)\)-plane. (b) shows that increasing either \((\beta K)^{-1}\) or \((\beta \kappa)^{-1}\) leads to melting of the crinkled phase.

FIG. 2. Renormalization flows Eqs. (14) and (15). (a) shows three-dimensional flows in \(x\), \(y\), and \(z\). (b) and (c) show, respectively, flows projected onto the \((y, z)\) and \((y, x)\) planes, which are similar to those in the \((y, x)\)-plane of a rigid flat surface.