$n$-atic Order and Continuous Shape Changes of Deformable Surfaces of Genus Zero

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Abstract

We consider in mean-field theory the continuous development below a second-order phase transition of $n$-atic tangent plane order on a deformable surface of genus zero with order parameter $\psi = \langle e^{in\theta} \rangle$. Tangent plane order expels Gaussian curvature. In addition, the total vorticity of orientational order on a surface of genus zero is two. Thus, the ordered phase of an $n$-atic on such a surface will have $2n$ vortices of strength $1/n$, $2n$ zeros in its order parameter, and a nonspherical equilibrium shape. Our calculations are based on a phenomenological model with a gauge-like coupling between $\psi$ and curvature, and our analysis follows closely the Abrikosov treatment of a type II superconductor just below $H_{c2}$.

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When aliphatic molecules are dissolved in water, they can spontaneously segregate into bilayer membranes in which hydrocarbon tails are shielded from contact with water. Depending on conditions, these membranes can form random, extended surfaces, regular periodic structures, or closed vesicles separating an interior from an exterior[1]. Membranes of a similar nature but with more structure and greater complexity form biological cell walls. In a wide class of membranes molecules move freely within the membrane forming a 2-dimensional fluid offering little resistance to changes in membrane shape. Such membranes are physical examples of random surfaces, which can undergo violent shape changes. Molecules in membranes can also exhibit varying degrees of orientational and positional order[2] including tilt, hexatic, and crystalline order similar to that found in free standing liquid crystal films [3]. These ordered membranes provide fascinating laboratories for the study of the coupling between order and geometry, analogous in many ways to the coupling between matter and geometry in general relativity. The underlying cause of this coupling is easy to see. A vector field (or any field describing orientational order) cannot be everywhere parallel if it is forced to lie on a surface, such as that of a sphere, that curves in two directions and thus has nonzero Gaussian curvature. It could lower its energy by flattening the surface. An additional complication arises when order develops on closed surfaces. A closed surface can be classified according to its genus (or number of handles) $g$: a sphere has genus zero, a torus genus one, etc. Orientational order on a closed surface necessarily [4] has topological defects (vortices) with total strength (vorticity) equal to the Euler characteristic $2(1-g)$ of the surface. Tangent plane order on a sphere will have vorticity 2, a torus vorticity 0, etc. The continuous development of vector order on a deformable surface of genus zero will be accompanied by a continuous change from spherical to ellipsoidal shape[5]. Since vortices are energetically costly, it may be favorable for a closed physical membrane to transform into an open cylindrical structure [6] when tangent plane order develops in response to changes in temperature or other control variable. Indeed, there are a number of experimental examples of shapes changes[7] that may be explained by the development of tangent plane order.

In this paper, we investigate in mean-field theory the development of $n$-atic order on a
closed surface of genus zero and the concomitant change in shape from spherical to non-spherical. An $n$-atic order parameter can have vortices of strength $1/n$, and, since it is generally favorable to form vortices of minimum strength, we expect $2n$ maximally separated vortices of strength $1/n$ to be present in the ordered phase. Thus for $n = 1$, we expect two antipodal vortices[5], and respectively for $n = 2$, $n = 3$ and $n = 6$, we expect vortices at the vertices of a tetrahedron, an octahedron, and an icosahedron. Indeed calculations on a rigid sphere confirm this conjecture[6,8]. We also expect the vesicle shape to change from spherical to ellipsoidal, tetrahedral, octahedral, or icosahedral in the four cases above. Fig. 1 shows our calculated shapes for temperatures just below the transition temperature to the $n$-atic state for $n = 1, 2, 3, 4,$ and $6$.

Our calculations are based on a phenomenological Hamiltonian[9] for a complex order parameter field whose coupling to shape occurs via a covariant derivative and via changes in the metric tensor. The model is almost identical to the Landau-Ginzburg theory of superconductivity except that vorticity is fixed by surface topology rather than energetically determined by an external magnetic field. The ordering transition we find is very similar to the transition from a normal metal to the Abrikosov vortex lattice[10] in a superconductor, and indeed our analysis follows very closely that of Abrikosov. We find the order parameter, which is necessarily spatially inhomogeneous because of the topological constraint on the total vorticity, from among a highly degenerate set of functions that diagonalize the harmonic Hamiltonian on a rigid sphere. This degenerate set has exactly $2n$ zeros at arbitrary positions on the sphere and is very similar in form to fractional quantum Hall wave functions[11].

Positions on a two-dimensional surface in $R^3$ are specified by a vector $\mathbf{R}(\sigma)$ as a function of a two-dimensional coordinate $\sigma = (\sigma_1, \sigma_2)$. Associated with $\mathbf{R}(\sigma)$ is a metric tensor $g_{ab}(\sigma) = \partial_a \mathbf{R}(\sigma) \cdot \partial_b \mathbf{R}(\sigma)$ and a curvature tensor $K_{ab}(\sigma)$ defined via $\partial_a \partial_b \mathbf{R} = K_{ab} \mathbf{N}$ where $\mathbf{N}$ is the local unit normal to the surface. To describe tangent-plane $n$-atic order, we introduce orthonormal unit vectors $\mathbf{e}_1$ and $\mathbf{e}_2$ at each point on the surface. If $\mathbf{t}(\sigma)$ is any unit tangent vector, then $\mathbf{e}_1(\sigma) \cdot \mathbf{t}(\sigma) = \cos \theta(\sigma)$ defines a local angle $\theta(\sigma)$. $n$-atic order is then described by the order parameter $\psi(\sigma) = \langle e^{in\theta(\sigma)} \rangle$, which can be related to the $n$th rank symmetric
traceless tensor constructed from the vector \( t \). Note that since \( \theta(\sigma) \) depends on the choice of orthonormal vectors \( e_1 \) and \( e_2 \), the order parameter \( \psi(\sigma) \) does as well. This means that any spatial derivatives in a phenomenological Hamiltonian for \( \psi \) must be covariant derivatives.

The long-wavelength Landau-Ginzburg Hamiltonian for \( \psi \) is \( \mathcal{H}_\psi = \mathcal{H}_1 + \mathcal{H}_2 \) where

\[
\mathcal{H}_1 = \int d^2 \sigma \sqrt{g} \left[ r |\psi|^2 + \frac{1}{2} u |\psi|^4 \right], \quad \mathcal{H}_2 = C \int d^2 \sigma \sqrt{g} g^{ab} (\partial_a - i A_a) \psi (\partial_b + i A_b) \psi^*,
\]

where \( A_a = e_1 \cdot \partial_a e_2 \) is the spin connection, \( g = \det g_{ab} \) and \( g_{ab} g^{bc} = \delta^c_e \). When \( n = 6 \), this \( \mathcal{H}_\psi \) is identical to the Hamiltonian for hexatic order on a deformable surface introduced in Ref. [12]. It is important to note that the covariant derivative \( D_a = \partial_a - i A_a \) depends on \( n \). The energy associated with shape changes of a constant area membrane is described by the Helfrich Hamiltonian[13],

\[
\mathcal{H}_{\text{curv}} = \frac{1}{2} \kappa \int d^2 \sigma \sqrt{g} (K^a_a)^2,
\]

The complete Hamiltonian for \( n \)-atic order on a deformable surface is \( \mathcal{H} = \mathcal{H}_\psi + \mathcal{H}_{\text{curv}} \).

We can now specialize to surfaces of genus zero with constant area \( \mathcal{A} = 4\pi R^2 \) whose shapes do not differ significantly from that of a sphere. We choose \( \sigma = (\theta, \phi) \equiv \Omega \) to be the polar coordinates of a sphere and set \( \mathbf{R}(\Omega) = R_0 [1 + \rho(\Omega)] \mathbf{e}_r \), where \( \mathbf{e}_r \) is the radial unit vector. This allows us to introduce reduced metric and curvature tensors \( \overline{g}_{ab} \) and \( \overline{K}_{ab} \) via \( g_{ab} = R_0^2 \overline{g}_{ab} \) and \( K_{ab} = R_0^{-1} \overline{K}_{ab} \). The field \( \rho(\Omega) \) measures deviations from sphericity and can be expanded in spherical harmonics. Any isotropic change in \( \mathbf{R} \) can be described by \( R_0 \). In addition, uniform translations, which change neither the shape or the energy of the vesicle, correspond to distortions in \( \rho \) with \( l = 1 \). These considerations imply that \( \rho \) will have no \( l = 0 \) or \( l = 1 \) components: \( \rho(\Omega) = \sum_{l=2}^\infty \sum_{m=-l}^l \rho_{lm} Y_l^m(\Omega) \). The shape and size of the vesicle are determined entirely by the parameters \( R_0 \) and \( \rho_{lm} \). The reduced tensors \( \overline{g}_{ab} \) and \( \overline{K}_{ab} \) do not depend on \( R_0 \). Therefore, \( R_0 \) can be expressed as a function of \( \mathcal{A} \) and \( \rho_{lm} \) via the relation

\[
\mathcal{A} = \int d\Omega \sqrt{\overline{g}} = R_0^2 \int d\Omega \sqrt{\overline{g}}.
\]

In the disordered phase \( \rho = 0 \), and \( R = R_0 \). We will use the Hamiltonian \( \mathcal{H} = \mathcal{H}_\psi + \mathcal{H}_{\text{curv}} \) expressed in terms of reduced parameters and the constant area \( \mathcal{A} \) in our calculations of shape changes below the second-order disordered-to-\( n \)-atic transition.
The similarities between $\mathcal{H}$ and the Landau-Ginzburg Hamiltonian for a superconductor in an external magnetic field,

$$\mathcal{H}_{\text{LG}} = \int d^3x |\psi|^2 + C|(|\nabla - ie^*A|\psi|^2 + \frac{1}{2}u|\psi|^4 + \frac{1}{8\pi}(\nabla \times A - \mathbf{H})^2],$$

are striking (Here $e^* = 2e/\hbar c$). Both have a complex order parameter $\psi$ with covariant derivatives providing a coupling between $\psi$ and a "vector potential" $A$ or $A_a$. In a magnetic field, the superconductor can undergo a 2nd order mean-field transition from a normal metal to the Abrikosov vortex lattice phase with a finite density of vortices determined energetically by temperature and the magnetic field $\mathbf{H}$. The magnetic field is conjugate to the vortex number $N_v$ since $\int d^3x (\nabla \times \mathbf{A}) = LN_v\phi_0$, where $L$ is the length of the sample along $\mathbf{H}$ and $\phi_0 = \hbar c/2e$ is the flux quantum. On a closed surface with $n$-atic order, there is a second-order mean-field transition to a state with vortex number determined by topology rather than conjugate external field. Thus, the $n$-atic transition on a closed surface is analogous to transition to an Abrikosov phase with a fixed number of vortices rather than fixed field conjugate to vortex number.

Before proceeding with our analysis of the $n$-atic transition on a deformable sphere, it is useful to recall Abrikosov’s calculation of the transition to the vortex state. The first step is to calculate the eigenfunctions of the Harmonic part of $\mathcal{H}_{\text{GL}}$ when $\nabla \times A = \mathbf{H}$. These can be divided into highly degenerate sets separated by an energy gap $\hbar \omega_c = 2Ce^*H$. In the Landau gauge with $A = (0, Hx, 0)$, the eigenfunctions in the lowest energy manifold are $\psi_k = e^{iky}e^{-e^*H(x-x_k)^2}$ where $x_k = k/e^*H$. The order parameter $\psi(x)$ of the ordered state is expressed as a linear combination $\psi(x) = \sum C_k \psi_k$ where the complex parameters $C_k$ are determined by minimization of $\mathcal{H}_{\text{GL}}$.

We will now proceed to analyze our problem in the same spirit. We first diagonalize $\mathcal{H}_2$ in the high-temperature spherical state when $\rho = 0$ and $A_\phi = A_\phi^0 = -\cos \theta, A_\theta = A_\theta^0 = 0$, i.e., we determine the functions $\psi$ that satisfy $CD_aD^a\psi = e^\psi$, for $\rho = 0 A_a = A_a^0$. In the lowest energy manifold, $\psi$ will have exactly $2n$ zeros specifying the positions of vortices of strength $1/n$. In the stereographic projection gauge where $z = \tan(\theta/2)e^{i\phi}$, we find
\[
\psi = \alpha \left( \frac{2|z|}{1 + |z|^2} \right)^n \frac{1}{z^n} \prod_{i=1}^{2n} (z - z_i),
\]
and \( \epsilon = Cn/R \). This function has zeros at the \( 2n \) points \( z_i \) and only at these points. Since these functions are polynomials in \( z \) multiplied by a common prefactor, any linear combination of them will yield another function of exactly the same form but with different positions of zeros. Thus, Eq. (4) is the most general function in the lowest energy manifold. We note the similarity between \( \psi^{1/n} \) and fractional quantum Hall wavefunctions[11]. Functions in higher energy manifolds will have more zeros corresponding to the creation of \( \pm \) vortex pairs. Reexpressing \( z \) and \( z_i \) in polar coordinates and choosing \( \alpha \) appropriately, we obtain
\[
\psi = \psi_0 \prod_{i=1}^{2n} \left( \sin \frac{\theta_i}{2} \cos \frac{\theta_i}{2} e^{i(\phi - \phi_i)/2} - \cos \frac{\theta_i}{2} \sin \frac{\theta_i}{2} e^{-i(\phi - \phi_i)/2} \right) \equiv \psi_0 P(\Omega)
\]
as a function of the polar coordinates \( \Omega_i = (\theta_i, \phi_i) \) of the positions of its zeros on a sphere.

Since \( \psi \) of Eq. (5) is the most general function in the lowest energy manifold, the order parameter and vesicle shape (determined by \( \rho \)) just below the transition are obtained by minimizing \( \mathcal{H} \) over \( \psi_0 \) and the positions of zeros. To order \( \psi^4 \), we can write \( \mathcal{H} \) as
\[
\mathcal{H} = \frac{A}{4\pi} \int d\Omega \left[ (r - r_c)|\psi|^2 + \frac{1}{2} u|\psi|^4 \right] + \int d\Omega \rho(\Omega) \Phi'(\Omega) + \frac{\kappa}{2} \sum l(l^2 - 1)(l + 2)|\rho_{lm}|^2,
\]
where \( r_c = -4\pi nC/A \) and
\[
\Phi'(\Omega) = (A/2\pi)(r|\psi|^2 + \frac{1}{2} u|\psi|^4) - \frac{1}{\sin \theta} \partial_a (\gamma_a^0 J^b) \equiv \psi_0^2 \Phi(\Omega)
\]
with \( J^b = g^{-1/2} \delta \mathcal{H}/\delta A_b \) evaluated at \( \rho_{lm} = 0 \) and \( R_0 = R \). Minimization over \( \rho \) and \( \psi_0 \) leads to \( \psi_0^2 = -r[\{\Omega_i\}]/u[\{\Omega_i\}] \),
\[
\rho_{lm} = -\frac{1}{\kappa l(l^2 - 1)(l + 2)} \int d\Omega \gamma^*_lm(\Omega) \Phi'(\Omega) \equiv -\frac{\psi_0^2}{\kappa l(l^2 - 1)(l + 2)} \Phi_{lm}(\Omega),
\]
and the effective free energy density,
\[
f[\{\Omega_i\}] = -\frac{1}{2} \frac{r^2[\{\Omega_i\}]}{u[\{\Omega_i\}]},
\]
depending only on the positions \( \{\Omega_i\} \) of the zeros of \( P(\Omega) \) where
\[ r\{\Omega_i\} = (r - r_c) \int d\Omega |P(\Omega)|^2, \]
\[ u\{\Omega_i\} = u \int d\Omega |P(\Omega)|^4 - \frac{4\pi}{\kappa A} \sum_{l,m} \frac{1}{l(l^2 - 1)(l + 2)} |\Phi_{lm}|^2. \]

The next step is to minimize \( f\{\{\Omega_i\}\} \) over \( \Omega_i \). Though in principle straightforward, this task becomes quite complicated as \( n \) grows large. In order to evaluate \( f\{\{\Omega_i\}\} \), it is necessary to integrate \( |P(\Omega)|^2 \) and \( |P(\Omega)|^4 \) over \( \Omega \) and to calculate \( \rho_{lm} \) for arbitrary \( \{\Omega_i\} \). The function \( |P(\Omega)|^2 \) can be expressed as \( \prod_2 n_i (1 - \cos \gamma_i) \) where \( \cos \gamma_i = \cos \theta \cos \theta_i + \sin \theta \sin \theta_i \cos(\phi - \phi_i) \).

Thus \( |P(\Omega)|^2 \) is a polynomial of order \( 3^{2n} \) in \( \cos \theta \) and \( \sin \theta \). \( |\Phi(\Omega)| \) is more complicated; it is a sum of \((n/2)(n + 1) + 1\) polynomials of order \( 3^{2n} \). We have been able to evaluate \( f\{\{\Omega_i\}\} \) analytically for \( n = 1 \) and \( n = 2 \) (where \( |P(\Omega)|^2 \) has 81 terms). For these two cases, we find, as expected that the minimum energy configurations are, respectively, those with zeros of \( |P(\Omega)| \) at opposite poles and at the vertices of a tetrahedron. For \( n > 2 \), a complete evaluation of \( f\{\{\Omega_i\}\} \) for arbitrary \( \{\Omega_i\} \) becomes a daunting task. We, therefore, appealed to symmetry to treat \( n = 3, 4 \) and 6. For \( n = 3 \) and \( n = 6 \), we expect the zeros of \( |P(\Omega)| \) to lie, respectively, at the vertices of an octahedron and an icosahedron. For \( n = 4 \), following the calculations of Palthy-Muhoray[8], we expect the zeros to lie at the vertices of a distorted cube obtained by rotating its top face about its four-fold axis by \( \pi/4 \) and compressing opposite faces. For this case, we minimized the energy over a single parameter determining the separation between opposite rotated faces.

The shape function \( \rho(\Omega) = \psi_0^2 \overline{p}^{(n)}(\Omega) \) associated with \( n \)-atic order is proportional to \( \psi_0^2 \sim r - r_c \) to the order of our calculations. In general, the Legendre decomposition of \( \overline{p}^{(n)} \) will contain Legendre polynomials of order \( 2n \). For \( n = 1, 2, \) and 3, we find

\[ \overline{p}^{(1)}(\Omega) = \frac{1}{4!} \frac{8}{3} \sqrt{\frac{\pi}{5}} Y_2^0 \]
\[ \overline{p}^{(2)}(\Omega) = \frac{1}{5!} \frac{80}{27} \sqrt{\frac{\pi}{7}} [Y_3^0 + \sqrt{\frac{2}{5}} (-Y_3^3 + Y_3^{-3})] + \frac{2!}{6!} \frac{16}{45} \sqrt{\pi} [Y_4^0 - \sqrt{\frac{10}{7}} (-Y_4^3 + Y_4^{-3})] \]
\[ \overline{p}^{(3)}(\Omega) = \frac{2!}{6!} \frac{12}{11} \sqrt{\pi} [Y_4^0 + \sqrt{\frac{5}{14}} (Y_4^4 + Y_4^{-4})] + \frac{4!}{8!} \frac{80}{3003} \sqrt{13\pi} [Y_6^0 - \sqrt{\frac{7}{2}} (Y_6^4 + Y_6^{-4})] \]

Fig. 1 shows the shapes described by these functions and the shapes \( n = 4 \) and \( n = 6 \) (whose shape functions are too long to display in this letter). The transformations from the
initial spherical shape to the distorted shapes occur continuously. Our calculations for the shape are valid to order $r - r_c$. As temperature is lowered, higher order terms in $r - r_c$ and higher order spherical harmonics are needed to describe the equilibrium shape. In Ref. [5], a variational function for $\psi$ and spherical harmonics up to order 8 were used to calculate the shape for $n = 1$ for temperature well below the transition. The shapes described by the functions in Eq. (11) exhibit unacceptable negative curvature regions at low temperature, and higher order spherical harmonics (with the appropriate symmetry) are needed to provide a correct description.

We have presented here an analysis of the mean-field transition to $n$-atic order on a fixed-area surface of genus zero. Our analysis is very similar to that of Abrikosov for the transition from a normal metal to a vortex lattice in a type II superconductor at $H_{c2}$ and completely ignores the effects of fluctuations, which may lead to qualitative changes in our results. We are really dealing with two kinds of order: $n$-atic order and the positional order of vortices. In mean-field theory, these two kinds of order develop simultaneously. In superconductors, fluctuations drive the normal-to-superconducting transition in a field first order[14]. In the Abrikosov phase, fluctuations of the vortex lattice destroy[15] superconductivity but not long-range periodic order. In two-dimensions, screening of vortices drive the Kosterlitz-Thouless transition in an infinite superconductor in zero field to zero[16]. Both the above effects may be important for $n$-atic order on a sphere, and we are currently investigating them.

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FIGURES

Mean-field shapes of deformable surfaces of genus zero with $n$-atic order. Above the mean-field transition temperature, the equilibrium shape is spherical for all $n$. Below, the transition, the equilibrium shape depends on $n$ and in general has a polyhedral form with $2n$ vertices that coincide with the positions of strength $1/n$ vortices.