Theoretical study of fluid membranes of spherical topology with internal degrees of freedom

R. M. L. Evans
Theoretical Physics Group, Department of Physics and Astronomy, The University of Manchester, Manchester M13 9PL, United Kingdom
(Received 27 July 1995)

A theoretical study of vesicles of topological genus zero is presented. The bilayer membranes forming the vesicles have various degrees of intrinsic (tangent-plane) orientational order, ranging from smectic to hexatic, that are frustrated by curvature and topology. The field-theoretical model for these "n-atic" surfaces has been studied before in the low temperature (mean-field) limit. The work presented here includes the effects of thermal fluctuations. Using the lowest Landau level approximation, the coupling between order and shape is cast in a simple form, facilitating insights into the behavior of vesicles. The order parameter contains vortices whose effective interaction potential is found and renormalized by membrane fluctuations. The shape of the phase space has a counterintuitive influence on this potential. A criterion is established whereby a vesicle of finite rigidity may be burst by its own in-plane order, and an analogy is drawn with flux exclusion from a type-I superconductor.

PACS number(s): 82.70.−y, 02.40.−k, 68.15.+e, 64.70.Md

I. INTRODUCTION

When amphiphilic molecules (those with hydrophobic and hydrophilic parts) are dissolved in water, they hide their aliphatic tails by grouping together and thus assemble themselves into structures. Depending on the geometry and chemistry of the particular surfactant, these structures may be anything from nanometer-scale mycils to macroscopic membranes arranged in stacks, bicontinuous networks of pipes, or closed surfaces. The literature on spontaneously self-assembling amphiphiles and biological and liquid-crystal membranes is vast. See, for example, [1, 2, or 3].

The research presented here is concerned with bilayer fluid membranes with internal orientational degrees of freedom. Fluidity of the membrane refers to the fact that molecules can move freely *within* the surface, although *perpendicular* deformations have an energy cost. The molecules have no positional crystalline order as the temperature is above the crystalline-to-fluid transition at which lattice dislocations proliferate. However, for some liquid crystals, this is not coincident with loss of *orientational* order, which occurs at a higher temperature. Various kinds of orientational order are possible. Liquid crystals in the smectic-C phase have carbon-chain tails which are tilted with respect to the local normal to the surface. The local mean direction of tilt, projected onto the local tangent plane of the membrane, gives a two-component vector order parameter, which disappears at the continuous transition to smectic-A phase, where rotational symmetry is restored [4]. Alternatively, the orientational order may be hexatic. In this case, the Kosterlitz-Thouless (KT) transition at which lattice disclinations proliferate, destroying the quasi-long-range hexagonal bond orientational order, is noncoincident with the lower temperature KT transition at which dislocations proliferate [5]. Nearest neighbor bond orientations give a basis for defining an order parameter, which again has two components in the local tangent plane. But a sixfold ambiguity in the choice of nearest neighbors arises from the local sixfold rotational invariance of the membrane. Mapping the local tangent plane onto the Argand plane, with some arbitrary direction chosen for the real axis, allows the two-component order parameter to be well defined as a complex number, thus

$$\psi(\boldsymbol{\sigma}) = \langle \exp[i6\Theta(\boldsymbol{\sigma})] \rangle ,$$

where $\boldsymbol{\sigma}$ is some two-component coordinate defined on the surface, and Θ is the bond angle with respect to an arbitrary coordinate axis. Notice that this definition is independent of which of the six bonds is chosen, since rotations of the membrane through $\pi/3$ correspond to a phase change of 2π in ψ, or an identity transformation. Hence, this two-component order parameter has the appropriate sixfold local rotational invariance. A similar complex order parameter can be defined for the smectic-C order described above. This has local full-turn invariance only, and magnitude ψ_0. Hence it may be mapped onto a complex field, thus

$$\psi_{\mathrm{C}}(\boldsymbol{\sigma}) = \langle \psi_0 \exp[i\Theta(\boldsymbol{\sigma})] \rangle ,$$

where Θ gives the orientation of the tail vectors projected onto the tangent plane. In each case, $\langle\,\rangle$ denotes a local thermal average. The notion may be generalized to an in-plane orientational order parameter with local n-fold rotational invariance being represented by a complex field

$$\psi(\boldsymbol{\sigma}) = \langle \psi_0 \exp[in\Theta(\boldsymbol{\sigma})] \rangle , \tag{1.1}$$

where Θ gives the orientation of one of the n principal directions of order. For smectic and bond-angle order in liquid crystals, $n \in \{1, 2, 4, 6\}$. Geometrical arguments

for this restriction on the possible orders of rotational symmetry are given in [6].

On a flat membrane, the continuous development of ψ is well modeled by a Ginzburg-Landau free energy functional of the form

$$\mathcal{H} = \int \{r|\psi|^2 + \tfrac{1}{2}u|\psi|^4 + C|\nabla\psi|^2\}\, d\mathcal{A}, \qquad (1.2)$$

where $d\mathcal{A}$ is an element of area, and r, u, and C are parameters of the particular conditions of the system being modeled.

On a flexible membrane, however, the free energy functional is a little more complicated. Let the membrane be treated as an ideal, two-dimensional, smooth surface. A Hamiltonian due to Helfrich [7] governs elastic deformations of an isotropic ($\psi = 0$) fluid membrane. This Hamiltonian is a functional of the intrinsic and extrinsic curvatures of the membrane, as defined below. Let $\boldsymbol{R}(\boldsymbol{\sigma})$ be the position vector in R^3 of a point on the surface with two-dimensional coordinate $\boldsymbol{\sigma} = (\sigma_1, \sigma_2)$. The surface has a metric tensor with components $g_{ab} = \partial_a \boldsymbol{R} \cdot \partial_b \boldsymbol{R}$, where a and b label the coordinates. The metric has inverse g^{ab} and determinant g. A covariant curvature tensor is defined by $K_{ab} = \boldsymbol{N} \cdot \partial_a \partial_b \boldsymbol{R}$, where $\boldsymbol{N}$ is the local unit normal. Note that dot products are evaluated in R^3. Using Einstein summation convention, and the metric and its inverse to lower and raise indices in the standard way, a more useful curvature tensor is defined thus: $K^a_b = g^{ac}K_{cb}$. Its determinant K is the Gaussian curvature of the surface, also called the intrinsic curvature, as it is experienced by "flatlanders" and other physical entities living within the two-dimensional world of the surface, who are oblivious to the way in which the surface is embedded in 3-space. Its trace K^a_a, however, is an extrinsic property, which cannot be determined by flatlanders. [The idea of "flatlanders" was used by E. A. Abbott in his book *Flatland* [8]. They are hypothetical beings who live in a two-dimensional space, and have no conception of a third dimension.] This quantity is known as the total curvature, or twice the mean curvature, and is the sum of the two principal radii of curvature of the surface at a given point [9]. Helfrich's Hamiltonian, describing the elastic properties of a constant area fluid membrane, can now be expressed as

$$\mathcal{H}_{\text{Helfrich}} = \int \{\tfrac{1}{2}\kappa(K^a_a)^2 + \kappa_G K\}\sqrt{g}\, d^2\sigma. \qquad (1.3)$$

Note that $\sqrt{g}\, d^2\sigma = d\mathcal{A}$. The phenomenological constants in this expression are the bending rigidity κ and the Gaussian curvature modulus κ_G. On a closed surface, the second term in Eq. (1.3) is a topological invariant, according to the Gauss-Bonnet formula

$$\int K\, d\mathcal{A} = 2\pi\chi,$$

where χ is the Euler number of the surface [10]. For an orientable surface of genus (number of "handles") G, the Euler number is given by

$$\chi = 2(1 - G).$$

Hence the dynamics of a membrane of given topology are not influenced by the second term of Eq. (1.3). What follows will concentrate on membranes of spherical topology (genus zero), so this term will be dropped.

The free energy functional governing the dynamics of n-atic fluid membranes cannot be found by simply adding together Eqs. (1.2) and (1.3), since (1.2) contains a gradient operator, which must be expressed in terms of coordinates which are no longer flat, but curvilinear. The derivatives in the flat-membrane expression $|\nabla\psi|^2 = \partial_x\psi^*\partial_x\psi + \partial_y\psi^*\partial_y\psi$ must be replaced by covariant derivatives thus: $|\nabla\psi|^2 = D^*_a\psi^* D^a\psi$, where D_a is of the form $\partial_a - inA_a$ with the connection $\boldsymbol{A}$ defined such that the free energy is invariant under general coordinate transformations. Clearly, $\boldsymbol{A}$ itself is not coordinate invariant, since ψ has coordinate dependence due to the arbitrariness of the reference axis for Θ in Eq. (1.1). There is some freedom in the choice of the gauge field $\boldsymbol{A}$. Here, $\boldsymbol{A}$ is chosen to be the "spin connection" $A_a = \boldsymbol{e}_1 \cdot \partial_a \boldsymbol{e}_2$, where $\boldsymbol{e}_b$ is a unit vector in the direction of $\partial_b \boldsymbol{R}$. Finally, we have the free energy functional for a closed, n-atic fluid membrane:

$$F[\psi(\boldsymbol{\sigma}), \boldsymbol{R}(\boldsymbol{\sigma})] = \int d^2\sigma\sqrt{g}\{r|\psi|^2 + \tfrac{1}{2}u|\psi|^4 + CD^*_a\psi^* D^a\psi + \tfrac{1}{2}\kappa(K^a_a)^2\} \qquad (1.4)$$

and, since the membrane's total area is fixed at $\mathcal{A}$ by the number of incompressibly packed constituent molecules, there is also a constraint

$$\int d^2\sigma\sqrt{g} = \mathcal{A}. \qquad (1.5)$$

The covariant derivatives provide a coupling between order and the shape of the membrane.

So far, the model and formalism are identical to that used by Park, Lubensky, and MacKintosh in their mean-field treatment of n-atic fluid membranes of genus zero (vesicles) [11]. They noted that, not only is n-atic ordering partly frustrated by curvature of its two-dimensional space, making parallelism impossible to achieve, but it is further frustrated by the spherical boundary conditions. Orientational order intrinsic to a surface of Euler number χ must have topological defects whose indices sum to χ. For instance, smectic-C (vector) order can form defects (sometimes called vortices) of index 1. Hence, on a sphere (Euler number 2) and in the absence of any antivortices (index-1 defects), there must be two defects in a Sm-C order parameter. At these poles, ψ vanishes smoothly to avoid infinite gradients. Clearly, an n-atic can form defects of index $1/n$ since it can rotate by less than a full turn in circling a pole, without its phase slipping. So n-atics form $2n$ vortices on a sphere, in the absence of excited vortex-antivortex pairs.

A similar approach to that of Park *et al.* will be used in this paper. The small deformations from sphericity of the n-atic fluid membrane are expressed as a real, scalar field, and the order parameter as a complex field ψ as described above. The shape deformation field is expanded in spherical harmonics, and ψ is expanded in eigenfunctions of the gradient operator. As an approximation,

the series expansion for ψ is truncated and only the degenerate set of lowest-eigenvalue functions are kept. The same approximation was used by Landau to find the wave function of an electron in a magnetic field [12], and by Abrikosov in his treatment of flux lattices in superconductors [13]. The study diverges from that of Park *et al.* when a simple expression is calculated for the coupling between the two fields. The free energy is cast into a form which allows the shape fluctuations to be integrated out exactly, giving renormalized coefficients for the order parameter. This effectively maps the deformable sphere problem onto a rigid sphere problem, which is soluble for the $n = 1$ case. In Sec. III, the stability of the system is analyzed to ascertain the conditions under which topological defects become too expensive, and are excluded from the membrane in a similar fashion to flux exclusion from a type-I superconductor. The partition function and various expectation values for $n = 1$ are calculated in Sec. VI, using some special symmetries of the problem. For other values of n, the system is not soluble, but approximate expectation values are found in Sec. VII, using diagrammatic expansion and the Hartree-Fock method, which gives correct results in the limit of high temperature.

II. CALCULATION

Using the expression $D_a = \partial_a - inA_a$, it is easy to show that, on a closed surface,

$$\int d^2\sigma \sqrt{g} D^a \psi D_a^* \psi^* \equiv - \int d^2\sigma \, \psi^* D_a(\sqrt{g} D^a \psi).$$

Both sides are real for all ψ; hence the operator $-g^{-1/2} D_a(\sqrt{g} D^a)$ is Hermitian. Eigenvalues of this operator scale as $\mathcal{A}$. A useful set of orthonormal basis functions is formed by normalized eigenfunctions of this operator on the unit sphere, where $\sqrt{g}\, d^2\sigma = d\Omega$, which is the usual solid angle element ($\sin\theta \, d\theta \, d\varphi$ in spherical polar coordinates). These functions are sometimes referred to as "Landau levels." There are $(2n+1)$ degenerate Landau levels with the lowest eigenvalue n. If ψ is expanded in this complete set of functions then, close to the mean-field phase transition, the partition function is dominated by configurations involving only the lowest Landau levels. Hence, in this regime it is a good approximation to expand ψ in these complex, degenerate lowest levels only. Thus the number of degrees of freedom in ψ is reduced to $2(2n+1)$, corresponding to freedom in the positions of the $2n$ vortices in the two-dimensional surface, together with an overall complex amplitude. On the unit sphere,

$$-\frac{D_a(\sqrt{g} D^a)}{\sqrt{g}} = -[\partial_\theta \partial_\theta + \operatorname{cosec}^2\theta \, \partial_\varphi \partial_\varphi + \cot\theta \, \partial_\theta + 2in \operatorname{cosec}\theta \cot\theta \, \partial_\varphi - n^2 \cot^2\theta]. \tag{2.1}$$

The lowest eigenfunctions of this operator and similar operators for other gauges are presented in different forms in [14,15], and [11], and are reexpressed here as

$$\phi_p = \sqrt{\frac{(2n+1)!}{4\pi(n+p)!(n-p)!}} \times \sin^{n+p}(\theta/2) \cos^{n-p}(\theta/2) \exp(ip\varphi) \tag{2.2}$$

for integer values of p between $-n$ and n. Any function ψ which is a linear combination of these functions obeys the relation

$$\partial_\theta \psi = [n \cot\theta - i \operatorname{cosec}(\theta) \, \partial_\varphi]\psi. \tag{2.3}$$

Let deviations from sphericity of the vesicle's shape be parametrized by a real, dimensionless, scalar field $\rho(\boldsymbol{\sigma})$ in the following way. If the ground-state vesicle shape is a sphere of radius R_0 then, with the origin at the center of the vesicle,

$$|\boldsymbol{R}(\boldsymbol{\sigma})| = [1 + \rho(\boldsymbol{\sigma})] \, R_0. \tag{2.4}$$

This is a "normal gauge" parametrization, and therefore carries *almost* the correct weight in a statistical ensemble [16]. This point will be readdressed later.

It will emerge that $\langle \rho^2 \rangle \sim \langle |\psi|^4 \rangle$. Equation (1.4) approximates the ψ potential by a series expansion, truncated at fourth order. Hence, it is consistent to also truncate to order ρ^2 and $|\psi|^2\rho$, i.e., the vesicles under consideration deviate little from spheres. To this order,

$$\sqrt{g}|\psi|^2 = R_0^2 \sin(\theta)(1 + 2\rho)|\psi|^2$$

and

$$-\psi^* D_a(\sqrt{g} D^a)\psi = n|\psi|^2 \sin\theta + 2n\psi^* \{ i\partial_\varphi \rho \, \partial_\theta \psi - i\partial_\theta \rho \, \partial_\varphi \psi + 2n \cos(\theta) \, \psi \, \partial_\theta \rho \}.$$

Applying the relation (2.3) and integrating by parts gives

$$\int -\psi^* D_a(\sqrt{g} D^a)\psi \, d^2\sigma = n \int d\Omega |\psi|^2 (1 - \nabla_\perp^2 \rho) + O(|\psi|^2 \rho^2),$$

where $\nabla_\perp^2 = [\partial_\theta \partial_\theta + \operatorname{cosec}^2(\theta) \, \partial_\varphi \partial_\varphi + \cot(\theta) \, \partial_\theta]$ is the covariant Laplacian. So the expression for the free energy becomes

$$F = R_0^2 \int d\Omega \{ (r - r_c)|\psi|^2 (1 + 2\rho) + \tfrac{1}{2} u |\psi|^4 + r_c |\psi|^2 (2 + \nabla_\perp^2)\rho \} + \mathcal{H}_{\text{Helfrich}} + O(|\psi|^6),$$

where

$$r_c \equiv -\frac{Cn}{R_0^2}.$$

It also emerges that $|\psi|^2 \sim (r - r_c)$ below the mean-field transition. See Sec. V for more explanation. Furthermore, from the definitions of K_a^a and ρ, it follows that

$$K_a^a = -\frac{2}{R_0}(1 - \rho - \tfrac{1}{2}\nabla_\perp^2 \rho + \rho^2 + \rho \nabla_\perp^2 \rho)$$

and, from Eq. (1.5),

$$\mathcal{A} = 4\pi R_0^2 + R_0^2 \int d\Omega \, \rho(1 + \tfrac{1}{2}\nabla_\perp^2)\rho,$$

since ρ and R_0 are defined in Eq. (2.4) in such a way that $\int \rho\, d\Omega \equiv 0$.

Hence, to $O(|\psi|^4)$, we may write

$$r_c = -\frac{4\pi n C}{\mathcal{A}}$$

and the free energy

$$F[\psi,\rho] = \int d\Omega \left[\frac{\mathcal{A}}{\triangle\pi} \left\{ (r - r_c)|\psi|^2 + \tfrac{1}{2}u|\psi|^4 \right\} - Cn|\psi|^2(2 + \nabla_\perp^2)\rho + \kappa \left\{ 2 + \rho\nabla_\perp^2\rho + \tfrac{1}{2}(\nabla_\perp^2\rho)^2 \right\} \right] \tag{2.5}$$

with the field ρ unaffected by the fixed area constraint to this order.

The coupling between the fields ψ and ρ, describing order and shape, has been cast into a very simple form, using some special properties of the lowest Landau levels of ψ in the spherical geometry. Note that a similar restriction has not been put on the phase space of ρ. All modes of shape fluctuation are available for small amplitude excitation. The remarkable simplicity of Eq. (2.5) is conducive to further exploration of the properties of n-atic vesicles, hitherto hindered by unwieldy notations.

It is clear from Eq. (2.5) that the mean-field transition temperature has been shifted from $r = 0$ to the lower temperature $r = r_c$ due to the nonzero lowest eigenvalue of the operator in Eq. (2.1) in the spherical geometry. Hence, ordering is frustrated by the curvature of the space.

Now let ρ be expanded in eigenfunctions of the covariant Laplacian $\nabla_\perp^2$. These functions are spherical harmonics Y_l^m, defined by

$$\nabla_\perp^2 Y_l^m = -l(l+1)Y_l^m.$$

The s-wave ($l = 0$) harmonic is not included in the series expansion, since this mode of deformation is already represented by rescaling R_0 in Eq. (2.4). The $l = 1$ modes are also excluded, as F will turn out to be independent of them. These three modes describe a positive deformation on one hemisphere of the vesicle, and negative on the opposite hemisphere. Hence, they simply correspond to the three degrees of translational freedom. The complex coefficients ρ_{lm} become the dynamical variables, where

$$\rho(\theta,\varphi) = \sum_{l=2}^{\infty} \sum_{m=-l}^{l} \rho_{lm} Y_l^m(\theta,\varphi).$$

The deformation field ρ is constrained to be real by demanding that

$$\rho_{lm}^* = (-1)^m \rho_{l-m},$$

which follows from the identity $Y_l^{m*} \equiv (-1)^m Y_l^{-m}$.

As stated earlier, the order parameter field ψ is expanded in the basis functions given in Eq. (2.2), thus

$$\psi = \sqrt{\frac{4\pi}{\mathcal{A}}} \sum_{p=-n}^{n} a_p \phi_p, \tag{2.6}$$

where a_p are $(2n+1)$ dimensionless, complex, dynamical variables.

The free energy can now be expressed in terms of the dynamical variables, thus

$$F = \alpha \sum_p a_p^* a_p + \sum_{p,q,r,s} \beta_{pqrs} a_p^* a_q^* a_r a_s + \sum_{p,q,l,m} \gamma_{pqlm} a_p^* a_q \rho_{lm} + \sum_{l,m} \Delta_l \rho_{lm}^* \rho_{lm}, \tag{2.7}$$

where

$$\alpha = r + \frac{4\pi n C}{\mathcal{A}}, \tag{2.8a}$$

$$\beta_{pqrs} = \frac{2\pi u}{\mathcal{A}} \int \phi_p^* \phi_q^* \phi_r \phi_s \, d\Omega, \tag{2.8b}$$

$$\gamma_{pqlm} = \frac{4\pi n C}{\mathcal{A}} (l+2)(l-1) \int \phi_p^* \phi_q Y_l^m \, d\Omega, \tag{2.8c}$$

$$\Delta_l = \tfrac{1}{2}\kappa l(l^2-1)(l+2), \tag{2.8d}$$

all of which coefficients are real. Indices run over the intervals $-n \le p,q,r,s \le n$ and $2 \le l < \infty$ and $-l \le m \le l$. Notice that, as stated earlier, $l = 1$ spherical harmonics contribute to neither the curvature energy nor the coupling, due to the factors of $(l-1)$.

Notice also that Eq. (2.7) is quadratic in the variables ρ_{lm}. Hence, in a partition function defined by

$$\mathcal{Z} = \int e^{-F(\{a_p\},\{\rho_{lm}\})} \mathcal{D}[\rho] \prod_q da_q^* da_q$$

the integral over all shapes may be done explicitly. But first, an explicit expression is needed for $\mathcal{D}[\rho]$. A naïve guess would be $\mathcal{D}[\rho]_{\text{naïve}} = \prod_{\boldsymbol{\sigma}} d\rho(\boldsymbol{\sigma})$, where the product is over all two-dimensional coordinates $\boldsymbol{\sigma}$. But this is incorrect. As explained in [16], there is a subtle geometrical factor which makes the measure nontrivial. Equation (2.4) is a normal gauge parametrization. Beginning from the reference of a sphere, the surface is deformed at each point *normal to itself* by an amount ρ, and each of the resulting surface configurations is counted with equal weight. Such a scheme is correct, but does not result from the naïve measure given above, for the following reason. Once the field ρ has a finite gradient, further increments $d\rho$ are no longer normal to the surface. They are, of course, normal to the *reference* surface, but that is not what we require. This is illustrated by Fig. 1, in which the reference surface S is deformed along the radial direction $\hat{\boldsymbol{r}}$ by an amount $R_0\rho$, to the surface S', and then by a further amount $R_0\delta\rho$ to the surface S''. The latter deformation is not in the direction of the normal $\boldsymbol{N}$ to surface S'. The correct measure is given by

$$\mathcal{D}[\rho] = \prod_{\Omega} \hat{\boldsymbol{r}} \cdot \boldsymbol{N} \, d\rho(\boldsymbol{\sigma}). \tag{2.9}$$

So the increment $d\rho$, in the direction of the normal to

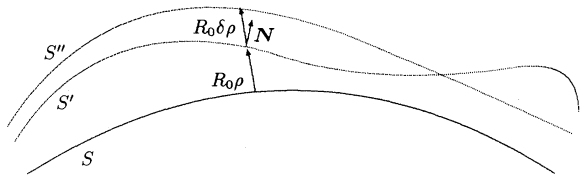


FIG. 1. Diagram illustrating that a normal displacement from surface S to S', when increased to S'', is no longer a normal displacement.

the reference surface, is projected onto the normal to the current surface by a dot product of the normals. This simple geometrical recipe given by Cai *et al.* [16] can be arrived at more rigorously by the tricky calculation of a Faddeev-Popov determinant. Note that the product in Eq. (2.9) must be taken over all coordinates in a coordinate-invariant way. It must be taken over all surface elements. To second order in ρ, this is equivalent to a product over all solid angles Ω. To this order,

$$\hat{\boldsymbol{r}} \cdot \boldsymbol{N} = 1 - \tfrac{1}{2}\left\{(\partial_\theta \rho)^2 + \operatorname{cosec}^2\theta(\partial_\varphi \rho)^2\right\}.$$

So the measure becomes

$$\mathcal{D}[\rho] = e^{\int \ln\left\{1-\frac{1}{2}[(\partial_\theta\rho)^2+\operatorname{cosec}^2\theta(\partial_\varphi\rho)^2]\right\}d\Omega} \prod d\rho$$

$$= e^{\frac{1}{2}\int d\Omega\, \rho\nabla_\perp^2\rho + \mathcal{O}(\rho^3)} \prod d\rho.$$

Hence the nontrivial part of the measure may be absorbed into the free energy, leaving the trivial measure $\prod_{lm} d\rho^*_{lm} d\rho_{lm}$. This is achieved by simply adding $\frac{1}{2}l(l+1)$ to the expression for Δ_l given in (2.8), which is equivalent to adding a correction to the value of κ, thus

$$\kappa \to \hat{\kappa} = \kappa + \frac{1}{(l-1)(l+2)}. \tag{2.10}$$

So taking due consideration of the measure has the effect of increasing the bending rigidity slightly for low harmonics. Since κ tends to be $\gg \frac{1}{4}$, and hence deformations are small in the systems under discussion, κ will generally be used instead of $\hat{\kappa}$ for ease of calculation in what follows. But the qualitative effects of the correction $(\hat{\kappa} - \kappa)$ will be assessed.

The deformational degrees of freedom ρ_{lm}, which appear quadratically in the free energy, can now be integrated out by completing the square, using the identity $\gamma_{pqlm} \equiv (-1)^m \gamma_{qpl-m}$. A new effective free energy, defined by

$$\mathcal{Z} = \int e^{-F^{\text{eff}}(\{a_p\})} \prod_q da_q^* da_q, \tag{2.11}$$

is found to be

$$F^{\text{eff}} = \alpha \sum_p a_p^* a_p + \sum_{p,q,r,s} \beta^{\text{eff}}_{pqrs} a_p^* a_q^* a_r a_s + \mathcal{H}_\rho, \tag{2.12}$$

where

$$\beta^{\text{eff}}_{pqrs} = \beta_{pqrs} - \frac{1}{4}\sum_{l=2}^{\infty}\sum_{m=-l}^{l} \frac{\gamma_{rqlm}\gamma_{pslm}}{\Delta_l} \tag{2.13}$$

and $\mathcal{H}_\rho$ is the free energy of shape fluctuations due to the Helfrich Hamiltonian alone, given by

$$\mathcal{H}_\rho = \sum_{l=2}^{\infty} \ln\left[\frac{1}{2}\left(\frac{\Delta_l}{\pi}\right)^{l+1}\right] = \zeta_1 \ln\kappa + \zeta_2,$$

where ζ_1 and ζ_2 are infinite constants in the continuum limit. This infinite part of the free energy will henceforth be renormalized away.

Consider for a moment the coefficients γ_{pqlm}, defined via the integral $\int \phi_p^* \phi_q Y_l^m d\Omega$. Now, the spherical harmonic $Y_l^m(\theta,\varphi)$ is of the form $P_l^m(\cos\theta)\exp(im\varphi)$, where P_l^m is an associated Legendre function, of the form $\sin^m\theta \sum_{k=0}^{l-m} b_k \cos^k\theta$ with constant coefficients b_k. The associated Legendre functions form a complete, orthogonal set of functions for each value of m. Note also that

$$\phi_p^*\phi_q \propto \sin^{p-q}\theta(1-\cos\theta)^{n+q}(1+\cos\theta)^{n-p}\exp i(q-p)\varphi.$$

It follows that it is possible to write the function $\phi_p^*\phi_q$ as a *finite* sum of spherical harmonics, i.e., with some constant coefficients c_k, it can be written $\phi_p^*\phi_q = \sum_{j=0}^{2n} c_j Y_j^{p-q*}$. Hence $\phi_p^*\phi_q$ is orthogonal to all spherical harmonics not included in this sum. So γ_{pqlm} vanishes for $l > 2n$, and the infinite sum in Eq. (2.13) can be replaced by a finite sum

$$\beta^{\text{eff}}_{pqrs} = \beta_{pqrs} - \frac{1}{4}\sum_{l=2}^{2n}\sum_{m=-l}^{l} \frac{\gamma_{rqlm}\gamma_{pslm}}{\Delta_l}. \tag{2.14}$$

Physically, this means that only the modes of deformation between $l = 2$ and $l = 2n$ couple to the lowest Landau levels of order.

III. STABILITY ANALYSIS

The original system of orientational order on a fluctuating sphere has now been mapped onto a rigid sphere problem, in which a_p are the only dynamical variables, by replacing the coupling β_{pqrs} by the effective coupling $\beta^{\text{eff}}_{pqrs}$, renormalized by shape fluctuations. The free energy closely resembles that of a superconducting film, penetrated normally by magnetic flux quanta, around which the supercurrent flows in vortices. It is well known [17] that changing the sign of the fourth-order term from positive to negative changes the nature of the superconductor from type II to type I, from which all flux vortices are excluded. The corresponding phenomenon of excluding all vortices from an n-atic vesicle appears impossible, since the vortices are topologically imperative. There is, in fact, an analogous exclusion of vortices, brought about by a catastrophic change in the vesicle's topology, at which point the model breaks down, since the order and deformation fields become large. In the analysis

of type-II superconductors, there is a similar breakdown of the model in the marginal limit. The criterion for a "type-I" vesicle is now found by a stability analysis.

The free energy of Eq. (2.12) is a function of the $(2n+1)$ complex variables a_p. It describes a stable system if F is large at infinity in all directions in the phase space, i.e., if $F \to +\infty$ as any linear combination of the variables a_p goes to infinity. Such a path to infinity may be parametrized by $a_p = \eta_p \Xi$, where $\Xi \to \infty$. The constants η_p define a phase-space direction and may be kept finite, without loss of generality, by the constraint $\sum_p \eta_p^* \eta_p = 1$. Substituting into Eq. (2.12) and neglecting quantities of less than fourth order in Ξ yields the criterion for stability

$$\sum_{p,q,r,s} \beta^{\text{eff}}_{pqrs} \eta_p^* \eta_q^* \eta_r \eta_s > 0 \quad \forall \{\eta_p\}.$$

There is one particular set of constants $\eta_p = \eta_p^0$ which minimizes this sum. This set definitely exists, due to the introduction of the constraint above. So the stability criterion may be expressed in terms of this specific set of constants, thus

$$\sum_{p,q,r,s} \beta^{\text{eff}}_{pqrs} \eta_p^{0*} \eta_q^{0*} \eta_r^0 \eta_s^0 > 0.$$

But this set of constants which minimizes the sum, subject to an overall magnitude constraint, is simply the set of *mean-field* (MF) values of a_p, multiplied by some scale factor. Hence the criterion for stability is $\sum \beta^{\text{eff}}_{pqrs} (a_p^* a_q^* a_r a_s)_{\text{MF}} > 0$, and may be written as

$$\int |\psi|^4_{\text{MF}} d\Omega > 4\pi\mu \sum_{l,m} \frac{(l+2)(l-1)}{l(l+1)} \left| \int |\psi|^2_{\text{MF}} Y_l^m d\Omega \right|^2 .$$

Let "malleability" μ be defined as the quantity $n^2 C^2 / \mathcal{A} u \kappa$, which is a measure of the ease with which the order may deform the vesicle. The marginal case, defining the crossover from type-II to type-I behavior, is given by $\mu = \mu_c$, where

$$\mu_c = \int |\psi|^4_{\text{MF}} d\Omega \Big/ 4\pi \sum_{l,m} \frac{(l+2)(l-1)}{l(l+1)} \times \left| \int |\psi|^2_{\text{MF}} Y_l^m d\Omega \right|^2 .$$

Using symmetry arguments to establish the mean-field configuration, $\mu_c(n)$ is found for the first two cases to be $\mu_c(1) = 9/4\pi$, $\mu_c(2) = 125/1567\pi$. For vesicles this malleable, the order parameter can deform the shape from a sphere to an intrinsically flat cylinder or polyhedron, and hence ordering is no longer frustrated by curvature. In other words, the vesicle bursts. This interpretation may not be the whole story, since the model breaks down as this instability is approached, due to the large magnitudes of the fields ψ and ρ. But it is clear that "ordinary" or type-II behavior is exhibited when $\mu < \mu_c$ and that a qualitatively different behavior, requiring a different model, exists in vesicles whose malleability is greater than this finite threshold.

Of course, use of the correct measure would give us a stability criterion for $\widehat{\kappa}$ instead of κ. According to Eq. (2.10), the corresponding condition on κ would be slightly less severe than calculated here. In other words, the effect of the nontrivial measure is to allow μ $(= n^2 C^2 / \mathcal{A} u \kappa)$ to be taken a little above μ_c before the vesicle bursts. This is because ignoring the measure leads to overcounting of the more deformed surfaces, and hence makes us overcautious about bursting the vesicle.

It will be demonstrated later that ordering increases and the region of temperature over which it arises sharpens with increasing malleability. The relationship between the magnitude of this order and the degree of shape deformation is now calculated.

IV. SHAPE CORRELATIONS

The original model for genus-zero vesicles with n-atic order, used by Park *et al.* [11], embodied in Eqs. (1.4) and (1.5), has been reduced to the much simpler form of Eq. (2.5) and all of the shape deformation degrees of freedom have been integrated out, leaving the effective free energy in Eq. (2.12), with coefficients calculable from Eqs. (2.14) and (2.8). Park *et al.* solved the model in the zero temperature limit (without fluctuations), and thus were able to produce diagrams of the vesicle shapes, from the fixed values of ρ_{lm} for each value of n. In reality of course, no such fixed values exist, as the shapes and vortex positions are in a constant state of flux, but expectation values of various moments of the variables ρ_{lm} and a_p can be calculated. The variables ρ_{lm} have been eliminated from the problem, so transformation equations must be found, relating their expectation values to those of a_p. This is done with the use of Eq. (2.7), and integrals of the form

$$\langle \rho_{lm} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}[\psi, \rho] \rho_{lm} e^{-F}$$

with the results

$$\langle \rho_{lm} \rangle = \frac{-1}{2\Delta_l} \sum_{p,q} \gamma_{pqlm} \langle a_p^* a_q \rangle \tag{4.1}$$

and

$$\langle \rho^*_{l_1 m_1} \rho_{l_2 m_2} \rangle = \frac{1}{4\Delta_{l_1}\Delta_{l_2}} \sum_{p,q,r,s} \gamma_{qrl_1 m_1} \gamma_{spl_2 m_2} \times \langle a_p^* a_q^* a_r a_s \rangle + \frac{\delta_{l_1 l_2} \delta_{m_1 m_2}}{\Delta_{l_1}}, \tag{4.2}$$

where δ_{xy} is the Krönecker delta. The expression for the second moment [Eq. (4.2)] is in two parts. The first represents deformations of the vesicle due to interaction with the order (i.e., ψ is attempting to align, and expel Gaussian curvature, except at the vortices where it is small). This part vanishes for higher spherical harmonics ($l > 2n$), which do not couple to the lowest Landau

levels. The second part represents uncorrelated deformations due to thermal excitation.

V. VALIDITY OF THE APPROXIMATIONS

Before proceeding further, an assessment is made of the regimes of validity of the approximations employed so far. The Ginzburg-Landau model carries with it an implicit approximation. It contains a truncated series expansion of the potential acting on ψ. For this to be valid, it is required that higher order terms in the expansion are smaller than lower order terms. This condition is satisfied at high temperature where ψ is small. It is also true at low temperature, provided that $(\mu_c - \mu) \gtrsim \pi^{-1}$. Clearly the model is good far from "critical malleability," as stated above.

In using the lowest-Landau-level approximation, it is assumed that the "ground-state" modes dominate the order parameter field. Let the expectation value of their coefficients be denoted $\langle a^*_{p_0} a_{p_0} \rangle$ and that of the next lowest level be denoted $\langle a^*_{p_1} a_{p_1} \rangle$. Then the ratio $\langle a^*_{p_1} a_{p_1} \rangle / \langle a^*_{p_0} a_{p_0} \rangle$ must be much less than unity. An order-of-magnitude estimate of this quantity is found from a high-temperature calculation to be $\sim \alpha/(\alpha - r_c)$, from which it follows that $|\alpha| \ll C/\mathcal{A}$. So this approximation is valid in the neighborhood of the mean-field transition. Let its region of validity cover a large domain in Figs. 1–4, so that all work presented here is correct. This requires that $C^2/\mathcal{A}u \gg (\mu_c - \mu)$.

One final approximation must be justified. In deriving Eq. (2.5), a factor $(1 + 2\rho)$ was dropped from the line above, with the explanation that $|\psi|^2 \sim (r - r_c)$, so this term was of too high an order in small quantities. This is only apparent at low temperature, but the derivation holds true at all temperatures for the following reasons. Replacing this lost factor is equivalent to multiplying γ_{pqlm} by $1 + 2(1 - \frac{r}{r_c})/(l+2)(l-1)$. Demanding that this is close to unity leads to the condition $|\alpha| \ll C/\mathcal{A}$, which is identical to the lowest-Landau-level criterion.

It remains only to calculate expectation values of the order-parameter field using Eq. (2.12). For $n = 1$ (vector order) this is done in Sec. VI by making use of various symmetries of the system. For other values of n, the calculation cannot be performed exactly, so a further approximation will be introduced in Sec. VII, where the problem is solved for general n. Either of these sections may be read without reference to the other.

VI. NONPERTURBATIVE SOLUTION FOR VECTOR ORDER

The $n = 1$ case (Sm-C order), solved at mean-field level in [4], has just two vortices on the spherical surface, and therefore has more symmetries than higher-n cases, which can be exploited in the solution of the integrals of Eq. (2.11).

A vesicle with vector order has two topologically required defects in the order parameter field. It is modeled using three complex dynamical variables, giving six degrees of freedom, corresponding to the positions of the two vortices in the two-dimensional space, plus an overall complex amplitude. Its energy is invariant under four obvious symmetries. The three Euler angles which relate to the spatial orientation of the vesicle are clearly irrelevant degrees of freedom, as is the complex phase of the overall amplitude of the order parameter field, which describes a global rotation of the orientation of in-plane order. The two remaining relevant dynamical quantities are the real amplitude of the order parameter and the geodesic distance between the vortices. A transformation of variables is now performed on Eqs. (2.11) and (2.12) to make these symmetries explicit.

Let us reexpress the lowest-Landau-level order in the form used in [11]:

$$\psi = \sqrt{\frac{12}{\mathcal{A}}}\psi_0 \prod_{k=1}^{2} \left[\sin\frac{\theta}{2} \cos\left(\frac{\theta_k}{2}\right) e^{i(\varphi-\varphi_k)/2} - \cos\frac{\theta}{2} \sin\left(\frac{\theta_k}{2}\right) e^{-i(\varphi-\varphi_k)/2} \right],$$

where (θ_k, φ_k) is the position of the kth vortex in spherical polar coordinates. The factor $\sqrt{12/\mathcal{A}}$ is convenient for the definition of the overall complex amplitude ψ_0. Equating this expression to Eq. (2.6) produces the transformation equations:

$$a_1 = 2\psi_0 \cos\frac{\theta_1}{2} \cos\left(\frac{\theta_2}{2}\right) e^{-i(\varphi_1+\varphi_2)/2}, \tag{6.1a}$$

$$a_{-1} = 2\psi_0 \sin\frac{\theta_1}{2} \sin\left(\frac{\theta_2}{2}\right) e^{i(\varphi_1+\varphi_2)/2}, \tag{6.1b}$$

$$a_0 = -\sqrt{2}\psi_0 \left[\cos\frac{\theta_1}{2} \sin\left(\frac{\theta_2}{2}\right) e^{i(\varphi_2-\varphi_1)/2} + \sin\frac{\theta_1}{2} \cos\left(\frac{\theta_2}{2}\right) e^{i(\varphi_1-\varphi_2)/2} \right], \tag{6.1c}$$

which relate the six dynamical variables $(a_{-1}, a^*_{-1}, a_0, a^*_0, a_1, a^*_1)$ to the new variables $(\psi_0, \psi^*_0, \theta_1, \theta_2, \varphi_1, \varphi_2)$. These transformation equations are now used to evaluate the terms of Eq. (2.12). It is found that $\sum_p a^*_p a_p = |\psi_0|^2[3 + \cos\theta_1 \cos\theta_2 + \sin\theta_1 \sin\theta_2 \cos(\varphi_1 - \varphi_2)]$. Let the positions of the vortices be expressed in a coordinate-invariant manner, by defining a unit vector $\boldsymbol{n}_k$ to point from the center of the vesicle towards the kth vortex. Then the cosine of the angle subtended by the vortices at the centre is $(\boldsymbol{n}_1 \cdot \boldsymbol{n}_2)$. In spherical polar coordinates, this becomes $\boldsymbol{n}_1 \cdot \boldsymbol{n}_2 = \cos\theta_1 \cos\theta_2 + \sin\theta_1 \sin\theta_2 \cos(\varphi_1 - \varphi_2)$. So this coordinate-invariant description has arisen naturally from the model, and the first term of Eq. (2.12)

becomes

$$\alpha \sum_{p=-1}^{1} a_p^* a_p = \alpha |\psi_0|^2 (3 + \boldsymbol{n}_1 \cdot \boldsymbol{n}_2).$$

Evaluation of the other terms of Eq. (2.12) is facilitated by noting that

$$|\psi|^2 = \frac{3}{\mathcal{A}} |\psi_0|^2 \prod_{k=1}^{2} (1 - \hat{\boldsymbol{r}} \cdot \boldsymbol{n}_k),$$

where $\hat{\boldsymbol{r}}$ is the unit vector in the direction of $\boldsymbol{R}$. Hence

$$\sum_{p,q,r,s} \beta_{pqrs}^{eff} a_p^* a_q^* a_r a_s = \frac{\mathcal{A}u}{8\pi} \int |\psi|^4 d\Omega - \frac{C^2}{3\kappa} \sum_{m=-2}^{2} \left| \int |\psi|^2 Y_2^m d\Omega \right|^2$$
$$= \frac{u|\psi_0|^4}{15\mathcal{A}} \left\{ 9 \left[13 + 10 \boldsymbol{n}_1 \cdot \boldsymbol{n}_2 + (\boldsymbol{n}_1 \cdot \boldsymbol{n}_2)^2 \right] - 4\pi\mu \left[3 + (\boldsymbol{n}_1 \cdot \boldsymbol{n}_2)^2 \right] \right\}.$$

As one would hope, all parts of the free energy are expressible in a coordinate-invariant way. To complete the transformation of variables in Eq. (2.11), a Jacobian must be evaluated. By calculation of a 6×6 determinant, it is established from the transformation Eqs. (6.1) that

$$\left| \frac{\partial(a_{-1}^*, a_{-1}, a_0^*, a_0, a_1^*, a_1)}{\partial(\psi_0^*, \psi_0, \theta_1, \theta_2, \varphi_1, \varphi_2)} \right| = |\psi_0|^4 (1 - \boldsymbol{n}_1 \cdot \boldsymbol{n}_2) \times \sin\theta_1 \sin\theta_2. \qquad (6.2)$$

Finally, let $\psi_0 = te^{i\sigma}$ so that t is a measure of the overall real amplitude of the order parameter. The partition function for smectic-C vesicles becomes

$$\mathcal{Z} = 2\pi \int e^{-F^{eff}(t, \boldsymbol{n}_1 \cdot \boldsymbol{n}_2)} t^5 (1 - \boldsymbol{n}_1 \cdot \boldsymbol{n}_2)\, d\Omega_1 d\Omega_2 dt,$$

where $d\Omega_k = \sin\theta_k d\theta_k d\varphi_k$. As noted above, the free energy is independent of the overall complex phase σ, which has been integrated out of the partition function, giving rise to the factor 2π. Integrals over both vortex positions still remain, although it is only their *relative* separation that is relevant. Let χ be a measure of this relative separation, being equal to the cosine of the angle subtended by the vortices at the center of the vesicle. Hence χ ranges in value from -1 when the vortices are antipodal to $+1$ when they are coincident. This variable is conveniently introduced into the partition function, thus

$$\mathcal{Z} = 2\pi \int e^{-F^{eff}(t, \boldsymbol{n}_1 \cdot \boldsymbol{n}_2)} t^5 (1 - \boldsymbol{n}_1 \cdot \boldsymbol{n}_2)\, dt\, d\Omega_1 d\Omega_2 \times \delta(\boldsymbol{n}_1 \cdot \boldsymbol{n}_2 - \chi) d\chi.$$

Hence

$$\mathcal{Z} = 16\pi^3 \int_{-1}^{1} d\chi \int_0^{\infty} dt\, t^5 (1 - \chi)\, e^{-F^{eff}(t,\chi)}, \qquad (6.3)$$

where $F^{eff} = A(\chi)t^2 + B(\chi)t^4$ with $A = \alpha(3 + \chi)$ and

$$B = \left\{ 9(13 + 10\chi + \chi^2) - 4\pi\mu(3 + \chi^2) \right\} / 15\omega^2.$$

The original set of six thermodynamic parameters $\{\mathcal{A}, r, u, C, \kappa\}$ has been reduced to just three independent combinations: (1) the shifted temperaturelike parameter $\alpha \equiv r + 4\pi nC/\mathcal{A}$, (2) the malleability $\mu \equiv n^2 C^2 / \mathcal{A} u \kappa$, and (3) the scale parameter $\omega \equiv \sqrt{\mathcal{A}/u}$, with $n = 1$ in this case.

Notice that there is more phase space available to vortices at large separations than to vortices in close proximity; a phenomenon arising from the phase space factor $(1 - \chi)$. One might naïvely predict that the thermal expectation value of χ would tend to zero in the limit of high temperature since the vortices would spend as much time close together as they would in opposite hemispheres. But this is not the case. The factor $(1 - \chi)$ favors large intervortex distances, and hence $\langle \chi \rangle$ must tend to a finite, negative number at high temperature.

The double integral of Eq. (6.3) is soluble, the method being given in Appendix A. The solution is

$$\mathcal{Z} = \frac{10\pi^{\frac{7}{2}} \omega^2}{(3 + 2\pi\mu)\alpha} \left[f\left(\frac{\alpha\omega}{\sqrt{\frac{4}{15}(9 - 4\pi\mu)}} \right) - f\left(\frac{\alpha\omega}{\sqrt{\frac{2}{15}(27 - 2\pi\mu)}} \right) \right], \qquad (6.4)$$

where $f(x) \equiv x\, e^{x^2} \operatorname{erfc} x$ and erfc is the complementary error function: $\operatorname{erfc} x = 1 - \operatorname{erf} x$. As $x \to +\infty$, $f(x) \to (1 - 1/2x^2)/\sqrt{\pi}$ and as $x \to -\infty$, $f(x) \to 2x\, e^{x^2}$.

From the expressions for the partition function in Eqs. (2.11) and (6.3), the following relations can be deduced:

$$-\frac{\partial \ln \mathcal{Z}}{\partial \alpha} = \langle (3 + \chi) t^2 \rangle = \left\langle \sum_p a_p^* a_p \right\rangle = \left\langle \int |\psi|^2 d\mathcal{A} \right\rangle, \qquad (6.5a)$$

$$\frac{5\omega^3}{6} \frac{\partial \ln \mathcal{Z}}{\partial \omega} = \langle (13 + 10\chi + \chi^2) t^4 \rangle, \qquad (6.5b)$$

$$\frac{15\omega^2}{4\pi} \frac{\partial \ln \mathcal{Z}}{\partial \mu} = \langle (3 + \chi^2) t^4 \rangle, \qquad (6.5c)$$

from which various correlators of the variables a_p are derived below. However, moments of χ cannot be found from $\mathcal{Z}$ alone and, as noted in Appendix A, it is not easy to simply invent a field coupled to χ to make this possible.

Expectation values of powers of χ are evaluated as follows. Returning to Eq. (6.3), the t integral alone is easily solved, giving

$$\mathcal{Z} = 2\pi^{\frac{7}{2}} \int_{-1}^{1} (1-\chi) B^{-\frac{3}{2}} f'\left(\frac{A}{2\sqrt{B}}\right) d\chi, \qquad (6.6)$$

where $f'(x)$ is the derivative of the function $f(x)$ defined above. Hence the moments of χ are given by

$$\langle \chi^m \rangle = \frac{2\pi^{\frac{7}{2}}}{\mathcal{Z}} \int_{-1}^{1} \chi^m (1-\chi) B^{-\frac{3}{2}} f'\left(\frac{A}{2\sqrt{B}}\right) d\chi,$$

which is a function of μ and $(\alpha\omega)$ only. A graph of $\langle\chi\rangle$ against $\alpha\omega$ is plotted in Fig. 2 for the cases of the rigid sphere ($\mu = 0$), the marginal type-I–type-II vesicle ($\mu = \mu_c$), and an intermediate malleability ($\mu = \mu_c/2$). As μ increases, the vesicle becomes less rigid, and the lower "kink" in the graph becomes sharper until, as $\mu \to 9/4\pi$, $\langle\chi\rangle$ tends to a singular function for which the mean-field value $\langle\chi\rangle = -1$ is correct for negative α, as the above integrands are then singular for this value of χ. In fact, it is generally true that mean field theory becomes increasingly accurate for negative α as μ approaches this critical value. The value $\mu_c = 9/4\pi$ is in agreement with the critical malleability calculated in Sec. III. For all μ, at high temperature (i.e., in the large $\alpha\omega$ limit), $\langle\chi\rangle$ tends to $5 - 8\ln 2 \approx -0.545$, which is a finite, negative number by virtue of the phase space factor discussed above. Consider Eq. (6.6) once more. Writing $\mathcal{Z} = \int d\chi \exp -V(\chi)$, we see that the effective intervortex potential,

$$V(\chi) = -\ln f'\left(\frac{A(\chi)}{2\sqrt{B(\chi)}}\right) + \tfrac{3}{2}\ln B - \ln(1-\chi)$$

is repulsive. For this reason, $\langle\chi\rangle \to -1$ in the low-temperature limit, as this is the antipodal configuration. Note that $V(\chi)$ is negatively dependent on μ. So the vortex-vortex repulsion is weakened when it is renormalized by shape fluctuations.

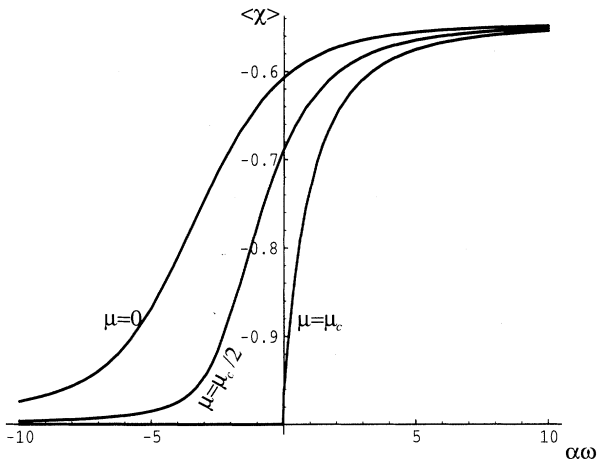


FIG. 2. Graph of the expectation value of the cosine of the angle subtended at the vesicle's center by the two vortices $\langle\chi\rangle$ against the temperaturelike combination $\alpha\omega$, for the cases $\mu = 0$ (the rigid sphere), $\mu = \mu_c$ (critical malleability), and $\mu = \mu_c/2$. The vortices are antipodal at low temperature, and tend to be well separated even at high temperature due to the shape of the phase space.

Let us return to the problem of calculating expectation values from the partition function as expressed in Eq. (6.4). Equations (6.5) may be used to find a certain set of expectation values, but these are not in the form required by Eqs. (4.1) and (4.2) for evaluating expectation values of the vesicle's shape. How are the correlators $\langle a_p^* a_q \rangle$ and $\langle a_p^* a_q^* a_r a_s \rangle$ to be deduced from the combinations of χ and t produced by Eqs. (6.5)? One can quickly convince oneself, from the form of Eq. (2.12), with its "momentum" conserving coupling, that $\langle a_p^* a_q \rangle = 0$ for $p \neq q$. Let $\mathcal{G}_p(t,\chi)$ be the mean value of $a_p^* a_p$, when thermally averaged over all configurations which have a particular value of t and χ. This constrained average is given by

$$\mathcal{G}_p(t_0,\chi_0) = \frac{\int a_p^* a_p \, e^{-F^{\text{eff}}} \delta(\chi-\chi_0)\,\delta(t-t_0) \prod_q da_q^* da_q}{\int e^{-F^{\text{eff}}} \delta(\chi-\chi_0)\,\delta(t-t_0) \prod_q da_q^* da_q}.$$

Using the Jacobian of Eq. (6.2) to change the variables of integration, the constrained average is found to be

$$\mathcal{G}_p(t_0,\chi_0) = \frac{1}{8\pi^2} \int a_p^* a_p \, \delta(\boldsymbol{n}_1 \cdot \boldsymbol{n}_2 - \chi_0) d\Omega_1 d\Omega_2.$$

And similarly, defining $\mathcal{G}_{pq}(t,\chi)$ to be given by thermally averaging $a_p^* a_p a_q^* a_q$ over all states of a given t and χ, it is found that

$$\mathcal{G}_{pq}(t_0,\chi_0) = \frac{1}{8\pi^2} \int a_p^* a_p a_q^* a_q \, \delta(\boldsymbol{n}_1 \cdot \boldsymbol{n}_2 - \chi_0) d\Omega_1 d\Omega_2,$$

all other fourth-order moments being zero. Having found these constrained averages, the full thermal averages of $a_p^* a_p$ and $a_p^* a_p a_q^* a_q$ will result from averaging the functions $\mathcal{G}_p(t,\chi)$ and $\mathcal{G}_{pq}(t,\chi)$ over t and χ. Hence, this is a derivation of transformation equations between correlators of a_p and correlators of t and χ. From Eqs. (6.5),

$$a_1^* a_1 = t^2(1+\cos\theta_1)(1+\cos\theta_2),$$

$$a_{-1}^* a_{-1} = t^2(1-\cos\theta_1)(1-\cos\theta_2),$$

$$a_0^* a_0 = t^2(1 - 2\cos\theta_1\cos\theta_2 + \boldsymbol{n}_1 \cdot \boldsymbol{n}_2).$$

So, in general, the integrals required are of the form

$\int g(\cos\theta_1,\cos\theta_2)\,\delta(\boldsymbol{n}_1\cdot\boldsymbol{n}_2-\chi)d\Omega_1 d\Omega_2$, where $g(x,y)$ is some function. This integral then, is of a function of the positions of two points on a unit sphere. The points are each varied over the surface in such a way that their separation remains constant. A general solution for such integrals is calculated in Appendix B. The solution is

$$\int g(\cos\theta_1,\cos\theta_2)\,\delta(\boldsymbol{n}_1\cdot\boldsymbol{n}_2-\chi)d\Omega_1 d\Omega_2 = 4\pi\int_0^1 ds\int_0^{2\pi} d\xi\,\frac{s}{\sqrt{1-s^2}}g(x,y),$$

where

$$\begin{aligned} x &= \tfrac{1}{2}s[(\sqrt{1+\chi}+\sqrt{1-\chi})\cos\xi \\ &\quad +(\sqrt{1+\chi}-\sqrt{1-\chi})\sin\xi], \\ y &= \tfrac{1}{2}s[(\sqrt{1+\chi}-\sqrt{1-\chi})\cos\xi \\ &\quad +(\sqrt{1+\chi}+\sqrt{1-\chi})\sin\xi]. \end{aligned}$$

Finally, the following correlation functions are found:

$$\langle a_p^* a_p\rangle = \langle t^2\rangle + \tfrac{1}{3}\langle t^2\chi\rangle = -\frac{1}{3}\frac{\partial \ln \mathcal{Z}}{\partial\alpha} \quad \forall p$$

and

$$\begin{aligned} \langle a_{-1}^* a_{-1} a_{-1}^* a_{-1}\rangle &= \langle a_1^* a_1 a_1^* a_1\rangle = 2\langle a_{-1}^* a_{-1} a_0^* a_0\rangle \\ &= 2\langle a_1^* a_1 a_0^* a_0\rangle = \tfrac{2}{15}(13\langle t^4\rangle + 10\langle t^4\chi\rangle + \langle t^4\chi^2\rangle) = \frac{\omega^3}{9}\frac{\partial \ln \mathcal{Z}}{\partial\omega}, \\ \langle a_{-1}^* a_{-1} a_1^* a_1\rangle &= \tfrac{2}{15}(3\langle t^4\rangle + \langle t^4\chi^2\rangle) = \frac{\omega^2}{2\pi}\frac{\partial \ln \mathcal{Z}}{\partial\mu}, \\ \langle a_0^* a_0 a_0^* a_0\rangle &= \langle a_{-1}^* a_{-1} a_1^* a_1\rangle + \tfrac{1}{2}\langle a_1^* a_1 a_1^* a_1\rangle. \end{aligned} \tag{6.7}$$

The derivatives are performed on Eq. (6.4). The order parameter is found to behave as follows:

$$\frac{1}{\omega}\left\langle\int|\psi|^2\,d\mathcal{A}\right\rangle = \frac{1}{\alpha\omega} - \left(\frac{f'\left(\frac{\alpha\omega}{\sqrt{\frac{4}{15}(9-4\pi\mu)}}\right)}{\sqrt{\frac{4}{15}(9-4\pi\mu)}} - \frac{f'\left(\frac{\alpha\omega}{\sqrt{\frac{2}{15}(27-2\pi\mu)}}\right)}{\sqrt{\frac{2}{15}(27-2\pi\mu)}}\right) \Bigg/ \left[f\left(\frac{\alpha\omega}{\sqrt{\frac{4}{15}(9-4\pi\mu)}}\right) - f\left(\frac{\alpha\omega}{\sqrt{\frac{2}{15}(27-2\pi\mu)}}\right)\right].$$

In the high-temperature limit, this tends to $3/\alpha\omega$ and, in the low-temperature limit, to the mean-field value of $-15\alpha\omega/(18-8\pi\mu)$. So, as μ increases towards the critical value of $\mu_c = 9/4\pi$, the order parameter increases in magnitude at low temperature, but not at high temperature, so the crossover between the two regimes becomes sharper, and mean-field theory becomes relatively more accurate. Figure 3 is a graph of the quantity $\langle\int|\psi^2|d\mathcal{A}\rangle\,(18-8\pi\mu)/15\omega$, which is normalized for low temperature, against $\alpha\omega$, for various values of the malleability μ.

The shape expectation values can now be found. As all of the correlators $\langle a_p^* a_p\rangle$ are equal, substituting for

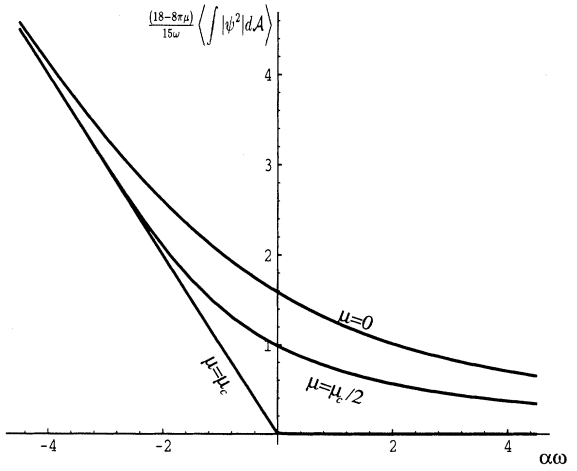


FIG. 3. Graph of the normalized order parameter $\frac{(18-8\pi\mu)}{15\omega}\left\langle\int|\psi^2|d\mathcal{A}\right\rangle$ against the temperaturelike quantity $\alpha\omega$, for various values of the malleability μ. As μ approaches the critical value $\mu_c = 9/4\pi$, low-temperature order increases, since the vesicle is intrinsically flattened, but high-temperature order is independent of μ. Hence mean-field theory becomes accurate in the marginal type-II–type-I limit, $\mu = \mu_c$.

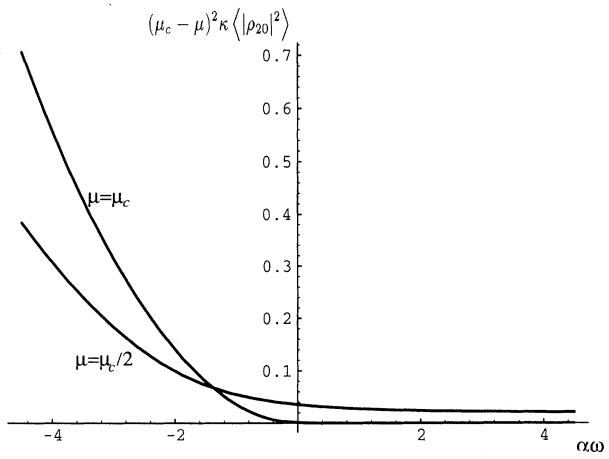


FIG. 4. Graph of the mean-square amplitude of the Y_2^0 mode of deformation multiplied by $(\mu-\mu_c)^2\kappa$, against the temperaturelike quantity $\alpha\omega$, for the cases $\mu = \mu_c/2$ and $\mu = \mu_c$.

$\langle a_p^* a_q \rangle$ in Eq. (4.1) with $\langle a_p^* a_p \rangle \delta_{pq}$ gives

$$\langle \rho_{lm} \rangle = \frac{-3\langle t^2 \rangle - \langle t^2 \chi \rangle}{6\Delta_l} \sum_p \gamma_{pplm}.$$

But $\sum_p \gamma_{pplm} = 0$. So all spherical harmonic amplitudes have a mean value of zero, despite the distorting influence of the two topological defects in ψ. This is because all vortex positions have been thermally averaged. The second moments of ρ are calculable, via Eq. (4.2), from the fourth moments of the order parameter field. For instance, the mean-square amplitude of the Y_2^0 deformation mode is found to obey

$$\kappa \langle |\rho_{20}|^2 \rangle = \frac{1}{12} + \frac{\pi}{45} \mu\alpha\omega \left(\frac{4[\frac{4}{15}(9-4\pi\mu)]^{-3/2} f'\left(\frac{\alpha\omega}{\sqrt{\frac{4}{15}(9-4\pi\mu)}}\right) - [\frac{2}{15}(27-2\pi\mu)]^{-3/2} f'\left(\frac{\alpha\omega}{\sqrt{\frac{2}{15}(27-2\pi\mu)}}\right)}{f\left(\frac{\alpha\omega}{\sqrt{\frac{4}{15}(9-4\pi\mu)}}\right) - f\left(\frac{\alpha\omega}{\sqrt{\frac{2}{15}(27-2\pi\mu)}}\right)} \right).$$

The constant $\frac{1}{12}$ is due to thermal excitation, and the other term arises from deformation by the in-plane order. As $\mu \to \mu_c$, this function goes to zero for positive α, and to $\frac{45}{128\pi^2}\left(\frac{\alpha\omega}{\mu_c - \mu}\right)^2$ for negative α. The latter expression tends to infinity as expected, since deformations become large as the marginal type-I–type-II case is approached. The function $(\mu_c - \mu)^2 \kappa \langle |\rho_{20}|^2 \rangle$, which is normalized for low temperature, is plotted against $\alpha\omega$ in Fig. 4 for the cases $\mu = \mu_c/2$ and $\mu = \mu_c$.

Notice that all of the measurable quantities calculated in this section are functions of μ and the combination $\alpha\omega$. Hence, temperature, measured from the mean-field transition, scales as ω^{-1}. So "transitions" from low- to high-temperature behavior become sharper for larger vesicles (i.e., when $\mathcal{A}$ is large compared with u).

VII. HARTREE-FOCK APPROXIMATION

Up to this point, the only approximation employed, other than the small amplitude approximations implicit in the Ginzburg-Landau model, has been the confinement of the order parameter field ψ to a $2(2n+1)$-dimensional phase space of the lowest eigenfunctions of the gradient operator. A further approximation is now introduced, in order to find expectation values of the n-atic order-parameter field for all of the values of n under consideration. The Hartree-Fock method will be used to produce an infinite, but incomplete, perturbation expansion, valid at high temperature — the opposite limit to that studied in [11].

Firstly, the bare, or Gaussian propagator h is calculated from the quadratic Hamiltonian

$$\mathcal{H}_0 = \alpha \sum_p a_p^* a_p$$

and is found to be independent of p,

$$\langle a_p^* a_q \rangle_0 \equiv \frac{\int a_p^* a_q e^{-\mathcal{H}_0} \prod_r da_r^* da_r}{\int e^{-\mathcal{H}_0} \prod_r da_r^* da_r} = \frac{\delta_{pq}}{\alpha} \equiv \delta_{pq} h_p.$$

Writing the free energy as $F = \mathcal{H}_0 + \mathcal{H}_1$ where $\mathcal{H}_1 = \sum_{p,q,r,s} \beta^{eff} a_p^* a_q^* a_r a_s$, the partition function becomes

$$\mathcal{Z} = \mathcal{Z}_0 \langle e^{-\mathcal{H}_1} \rangle_0,$$

where $\mathcal{Z}_0$ is the partition function for the quadratic Hamiltonian and $\langle \rangle_0$ indicates a thermal average with respect to this Hamiltonian. Hence, the renormalized propagator (i.e., the full thermal average) can be written as

$$\tilde{h}_p \equiv \langle a_p^* a_p \rangle = \frac{\langle a_p^* a_p e^{-\mathcal{H}_1} \rangle_0}{\langle e^{-\mathcal{H}_1} \rangle_0}.$$

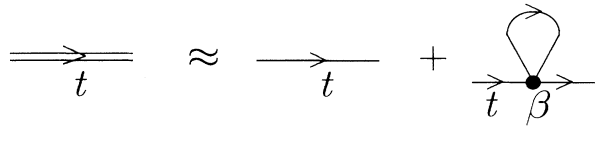
Taylor-expanding the exponentials and applying Wick's theorem, the terms in this formula may be represented by connected, two-leg graphs of all possible topologies, in which directed lines represent the bare propagators with "momentum" p, and the four-point vertices each carry a factor of β^{eff}. Momentum is conserved at the vertices, since β^{eff}_{pqrs} vanishes if $p + q \neq r + s$. The numerator is the sum of all connected and disconnected two-leg graphs, but the disconnected parts cancel with the denominator, which is the sum of all zero-leg graphs. This explanation is brief, since the Feynman-diagram expansion is given in many standard texts [18].

Truncating the expansion at one-loop graphs yields

$$\tilde{h}_t \approx h_t - \sum_{p,q,r,s}^{\text{connected}} \beta_{pqrs} \langle a_t^* a_p^* a_q^* a_r a_s a_t \rangle_0$$

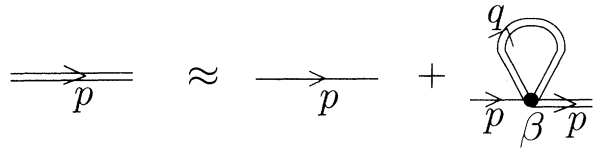
$$= h_t - \sum_{pqrs}^{\text{connected}} \beta_{pqrs} h_t h_p h_q (\delta_{tr} + \delta_{ts})(\delta_{pr}\delta_{qs} + \delta_{ps}\delta_{qr})$$

represented by



where a double line represents a renormalized propagator.

The Hartree-Fock scheme renormalizes the bare propagator with not just one loop diagram, but an infinity of diagrams belonging to a certain topological family. In particular, all those diagrams containing loops which do not span a vertex. This approximation to the renormalized propagator is defined implicitly by the equation



which can be thought of as iteratively replacing every bare propagator with the one-loop correction. The scheme generates graphs with the correct counting factors [17]. This pictorial equation corresponds to

$$\widetilde{h}_p \approx h_p \left(1 - 2\widetilde{h}_p \sum_q (\beta^{eff}_{pqqp} + \beta^{eff}_{pqpq})\widetilde{h}_q\right),$$

a set of $(2n+1)$ second order coupled polynomial equations. These generate many spurious solutions. But it is observed from calculation of β^{eff}_{pqrs} that $\sum_q(\beta^{eff}_{pqqp}+\beta^{eff}_{pqpq})$ is independent of p, and hence there is always a solution for which the $(2n+1)$ quantities $\widetilde{h}_p$ are equal, and positive. Henceforth, let $\widetilde{h}_p = \widetilde{h}\ \forall p$. This physical solution is given by the quadratic equation

$$\widetilde{h}^2\left(2\sum_q(\beta^{eff}_{pqqp} + \beta^{eff}_{pqpq})\right) + \alpha\widetilde{h} - 1 = 0 \qquad \forall p. \quad (7.1)$$

The coefficient of $\widetilde{h}^2$ is now calculated.

First,

$$\sum_q \beta^{eff}_{pqqp} = \frac{2\pi u}{\mathcal{A}}\int \phi_p^*\phi_p \sum_q \phi_q^*\phi_q d\Omega - \frac{8\pi^2 n^2 C^2}{\mathcal{A}^2\kappa} \times \sum_{l=2}^{2n}\sum_m \frac{(l+2)(l-1)}{l(l+1)} \times \int \phi_p^*\phi_p Y_l^m d\Omega \int Y_l^{m*}\sum_q \phi_q^*\phi_q d\Omega.$$

The function $\sum_{q=-n}^{n}|\phi_q|^2$, which appears twice in the above equation, may be written as

$$\frac{(2n+1)!}{4\pi}\sum_{r=0}^{2n}\frac{\sin^{2r}\left(\frac{\theta}{2}\right)\cos^{2(2n-r)}\left(\frac{\theta}{2}\right)}{r!(2n-r)!},$$

which is in the form of a binomial expansion of $\sin^2(\frac{\theta}{2}) + \cos^2(\frac{\theta}{2})$. It is therefore just a constant, $\sum_q|\phi_q|^2 = (2n+1)/4\pi$, and hence orthogonal to all non-s-wave spherical harmonics. It follows that

$$\sum_q \beta^{eff}_{pqqp} = (n+\tfrac{1}{2})\frac{u}{\mathcal{A}}.$$

Second, the sum $\sum_q \beta^{eff}_{pqpq}$ is found. This also has two parts, deriving from Eq. (2.14), and the first has already been calculated, since $\beta_{pqpq} = \beta_{pqqp}$. However, the order of indices is relevant to the second part, which does not vanish this time. There is no obvious method for simplifying this part, so the integrals have been calculated as required for each value of n of interest, with the result that

$$\sum_q(\beta^{eff}_{pqqp} + \beta^{eff}_{pqpq}) = (2n+1)\frac{u}{\mathcal{A}} - \frac{8\pi n^2 C^2}{\mathcal{A}^2\kappa}f(n),$$

where $f(1) = \frac{1}{12}$, $f(2) = \frac{43}{120}$, $f(4) = \frac{5471}{5040}$ and $f(6) = \frac{1376527}{720720}$. So the solution to Eq. (7.1) is

$$\frac{\varepsilon\widetilde{h}}{2\omega} \approx -\frac{\alpha\omega}{\varepsilon} + \sqrt{\frac{\alpha^2\omega^2}{\varepsilon^2}+1} \qquad \forall p, \quad (7.2)$$

where

$$\varepsilon \equiv 4\sqrt{n+\tfrac{1}{2} - 16\pi f(n)\mu}\ .$$

As before, μ is the malleability, $n^2C^2/\mathcal{A}u\kappa$, and ω is the scale parameter, $\sqrt{\mathcal{A}/u}$. From the definitions, the magnitude of the order parameter is

$$\int |\psi|^2 d\mathcal{A} = \sum_p \widetilde{h}_p = (2n+1)\widetilde{h}.$$

In Fig. 5, a graph of $\varepsilon\widetilde{h}/\omega$ against $\alpha\omega/\varepsilon$ is plotted in bold. Recall that α is a temperaturelike variable, measured with respect to the shifted mean-field transition temperature r_c. The figure shows that, within the lowest Landau level, and Hartree-Fock approximation schemes, the transition is removed. Instead, there is a gradual change from a low-temperature region with a high degree of order, to a poorly ordered high-temperature region, and this picture may be closer to the truth. Of course, the Hartree-Fock approximation should only be trusted at high temperature ($\alpha\omega/\varepsilon \gg 1$), as it is rigorously correct to $O(u)$. At low temperature, Eq. (7.2) tends asymptotically to $\widetilde{h} = -\alpha\omega^2/[n+\frac{1}{2} - 16\pi f(n)\mu]$, which is at variance with the correct mean-field expression $\widetilde{h} \to -\alpha/6\beta^{eff}_{0000}$. For $n = 1$, the former expression becomes $-3\alpha\omega^2/(18-16\pi\mu)$ and the latter $-5\alpha\omega^2/(18-8\pi\mu)$. Nonetheless, the Hartree-Fock expression is a useful qualitative indicator of the system's behavior. For comparison, the correct, lowest-Landau-level solution for $n = 1$, as calculated in Sec. VI, is plotted as dashed lines in Fig. 5, for various values of the malleability μ. Note that some μ dependance is contained in the function ε, which scales the axes of the figure. It is apparent from the graphs that the Hartree-Fock solution is correct at high temperature, and fairly poor at low temperature, except for the special case when $\mu = 9/14\pi$, for which the asymptotic gradient is in agreement with the mean-field value.

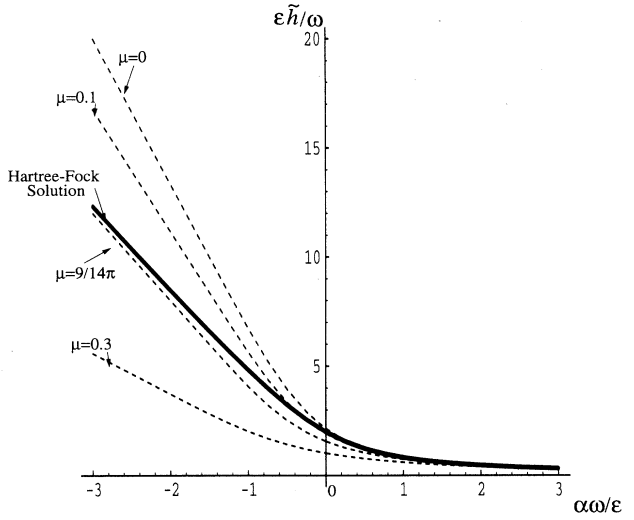


FIG. 5. Graph of $\tilde{\varepsilon h}/\omega$ against $\alpha\omega/\varepsilon$, showing the nonsingular progression from the low-temperature, highly ordered state to the high-temperature, poorly ordered state. The Hartree-Fock solution is shown as a continuous, bold line. For comparison, the more accurate solution for $n = 1$, as calculated nonperturbatively in Sec. VI, is shown dashed, for various values of the malleability μ.

The ordinate of Fig. 5 is a measure of the order parameter, under some normalization, while the abscissae is the temperature parameter α in units of ε/ω. Hence it is immediately apparent for the expression for ω that the crossover between high- and low-temperature regimes is sharper on larger vesicles. The crossover apparently becomes infinitely sharp at a finite value of the malleability, when $\mu = \mu_c = (2n+1)/[32\pi f(n)]$. Once again, it is apparent, from reference to the correct values of μ_c calculated in Sec. III, that the Hartree-Fock approximation gives qualitatively correct but quantitatively inaccurate results.

The shape expectation values can now be found. Substituting for $\langle a_p^* a_q \rangle$ in Eq. (4.1) with $\tilde{h}\delta_{pq}$ gives

$$\langle \rho_{lm} \rangle = \frac{-\tilde{h}}{2\Delta_l} \sum_p \gamma_{pplm}.$$

But $\sum_p \gamma_{pplm} = 0$. So all spherical harmonic amplitudes have a mean value of zero, despite the distorting influence of the $2n$ topological defects in ψ. This is because all vortex positions have been thermally averaged. The second moments are found, via Eq. (4.2), from the fourth moments of the order parameter field. From Wick's theorem, $\langle a_p^* a_q^* a_r a_s \rangle = (\delta_{pr}\delta_{qs} + \delta_{ps}\delta_{qr})\tilde{h}^2$. So Eq. (4.2) becomes

$$\langle \rho^*_{l_1 m_1} \rho_{l_2 m_2} \rangle = \frac{\tilde{h}^2}{4\Delta_{l_1}\Delta_{l_2}} \sum_{p,q} \gamma_{qpl_1 m_1}\gamma_{qpl_2 m_2} + \frac{\delta_{l_1 l_2}\delta_{m_1 m_2}}{\Delta_{l_1}}.$$

For instance, the autocorrelation function $\langle |\rho_{20}|^2 \rangle$ for $n = 1$ is evaluated as

$$\langle |\rho_{20}|^2 \rangle = \frac{1}{12\kappa}\left(\frac{4\pi\mu}{5\omega^2}\tilde{h}^2 + 1\right).$$

Hence deformations increase with the magnitude of the order parameter, as expected.

VIII. CONCLUSION

A simple expression has been derived for the coupling between the lowest Landau levels of intrinsic n-atic order and the shape of a genus-zero membrane. It has been shown, within the lowest-Landau-level approximation scheme, that all spherical harmonic amplitudes of deformations of such a vesicle have zero thermal average, but that their mean squares have a contribution from deformation by the order, and a contribution from thermal excitation. Only a finite number of spherical harmonics are coupled to the lowest Landau levels of order. It has been established that this order is capable of fundamentally altering, and perhaps bursting, a vesicle of finite rigidity. This occurs at a critical value of the malleability, for which the model is strongly analogous to that of a marginal type-I–type-II superconductor. As this critical value is approached, mean-field theory becomes increasingly accurate. The model for fluid vesicles with vector order has been solved exactly, using no further approximations, and the general result is established that the crossover from high- to low-temperature behavior becomes sharper for larger vesicles. The solution also confirms that mean-field theory becomes increasingly accurate as the critical malleability is approached. The counterintuitive result is ascertained that the two topological defects in the order are more likely to be found far apart than close together, even at high temperature, as the phase space volume element increases with defect separation. The Hartree-Fock approximation is valid at high temperature and significantly inaccurate at low temperature, but exhibits qualitatively correct behavior.

ACKNOWLEDGMENTS

Many thanks to Mike Moore for his contribution to this research. The work was funded by EPSRC Award No. 92310214.

APPENDIX A: SOLUTION OF THE PARTITION FUNCTION DOUBLE INTEGRAL

The integral required in Eq. (6.3) is

$$I = \int_{-1}^{1} d\chi(1-\chi) \int_0^\infty t^5 e^{-(At^2+Bt^4)} dt,$$

where $A = a(\chi+3)$ and $B = b(\chi^2+10\chi+13) - c(\chi^2+3)$. Expanding the first exponential as a sum and using $\int_0^\infty t^{2m+5} e^{-Bt^4} dt = \Gamma(\frac{m+3}{2})/4B^{\frac{m+3}{2}}$ gives

$$I = \frac{1}{4}\sum_{m=0}^{\infty}\frac{(-a)^m}{m!}\Gamma\left(\frac{m+3}{2}\right)\int_{-1}^{1}\frac{(1-\chi)(\chi+3)^m}{B^{\frac{m+3}{2}}}d\chi.$$

Using the indefinite integral

$$\int_{-1}^{1}\frac{(1-\chi)(\chi+3)^{2n-1}}{B^{n+1}}d\chi = \frac{-(3+\chi)^{2n}}{2n(2b+3c)B^n} + \text{const}$$

gives

$$I = \frac{1}{4}\sum_{m=0}^{\infty}\frac{(-a)^m(\frac{m+1}{2})!}{(m+1)!(2b+3c)} \times\left[\frac{1}{(b-c)^{\frac{m+1}{2}}} - \left(\frac{4}{6b-c}\right)^{\frac{m+1}{2}}\right].$$

The exact form of the function $B(\chi)$ is crucial to the solubility of the indefinite integral above. In particular, it is not easy to invent new fields coupled to the dynamical variables to aid computation of their expectation values. Now, applying the identity $(\frac{m}{2})!/m! \equiv \sqrt{\pi}/2^m(\frac{m-1}{2})!$ allows the infinite sum to be separated into the standard forms of exponentials and confluent hypergeometric functions, thus

$$I = \frac{1}{16(2b+3c)}\left[\frac{2\sqrt{\pi}}{\sqrt{b-c}}\exp\left(\frac{a^2}{4(b-c)}\right) - \frac{4\sqrt{\pi}}{\sqrt{6b-c}}\exp\left(\frac{a^2}{6b-c}\right) + \left(\frac{8a}{6b-c}\right){}_1F_1\left(1,\frac{3}{2};\frac{a^2}{6b-c}\right) - \left(\frac{2a}{b-c}\right){}_1F_1\left(1,\frac{3}{2};\frac{a^2}{4(b-c)}\right)\right].$$

The identities ${}_1F_1(a,c;x) \equiv e^x\,{}_1F_1(c-a,c;-x)$ and $\operatorname{erf}(x) \equiv \frac{2x}{\sqrt{\pi}}\,{}_1F_1(\frac{1}{2},\frac{3}{2};-x^2)$ are used [19] to give the result

$$I = \frac{\sqrt{\pi}}{4a(2b+3c)}\left[x\,e^{x^2}\operatorname{erfc} x\right]_{x=\frac{a}{\sqrt{6b-c}}}^{\frac{a}{\sqrt{4b-4c}}},$$

where erfc is the complementary error function: $\operatorname{erfc} x = 1 - \operatorname{erf} x$.

APPENDIX B: SOLUTION OF THE CONSTRAINED, TWO-POINT, SPHERICAL SURFACE INTEGRAL

The integrals required for thermally averaging combinations of a_p over states of a given t and χ are of the form

$$J = \int g(\cos\theta_1,\cos\theta_2)\,\delta(\boldsymbol{n}_1\cdot\boldsymbol{n}_2-\chi)d\Omega_1 d\Omega_2,$$

where $g(x,y)$ is some function. The integral is over the positions of two points on a unit sphere. The unit vectors $\boldsymbol{n}_1$ and $\boldsymbol{n}_2$ point from the center of the sphere to the points, each of which is varied over the surface, in such a way that $\boldsymbol{n}_1\cdot\boldsymbol{n}_2$ has the constant value χ. In spherical polar coordinates, the solid angle elements are $d\Omega_k = d(\cos\theta_k)d\varphi_k$. Hence

$$J = \int_{-1}^{1}d(\cos\theta_1)\int_{-1}^{1}d(\cos\theta_2)\,g(\cos\theta_1,\cos\theta_2) \times\int_0^{2\pi}d\varphi_1\int_0^{2\pi}d(\varphi_1-\varphi_2)\,\delta(\cos\theta_1\cos\theta_2+\sin\theta_1\sin\theta_2\cos(\varphi_1-\varphi_2)-\chi)$$

and

$$\int_0^{2\pi}d\varphi\,\delta(\cos\theta_1\cos\theta_2+\sin\theta_1\sin\theta_2\cos\varphi-\chi) = 2\int_{-1}^{1}\frac{d(\cos\varphi)}{\sin\theta_1\sin\theta_2\sin\varphi}\delta(\cos\theta_1\cos\theta_2+\sin\theta_1\sin\theta_2\cos\varphi-\chi) = \frac{2\Theta\left(\left[\frac{\chi-\cos\theta_1\cos\theta_2}{\sin\theta_1\sin\theta_2}\right]^2\right)}{\sqrt{\sin^2\theta_1\sin^2\theta_2-(\chi-\cos\theta_1\cos\theta_2)^2}},$$

where $\Theta(x)$ is the Heaviside step function, $\Theta(x<0)=0$, $\Theta(x>0)=1$. Now, setting $x=\cos\theta_1$ and $y=\cos\theta_2$ gives

$$J = 4\pi\int_{-1}^{1}dx\int_{-1}^{1}dy\frac{g(x,y)}{\sqrt{(1-x^2)(1-y^2)-(\chi-xy)^2}} \times\Theta\left(\frac{(\chi-xy)^2}{(1-x^2)(1-y^2)}\right).$$

The region of the xy plane for which the Heaviside function has a positive argument is the interior of an ellipse, contained within the unit square of integration. The transformation

$$2x = (\sqrt{1+\chi}+\sqrt{1-\chi})u + (\sqrt{1+\chi}-\sqrt{1-\chi})v,$$
$$2y = (\sqrt{1+\chi}-\sqrt{1-\chi})u + (\sqrt{1+\chi}+\sqrt{1-\chi})v,$$

with Jacobian

$$\frac{\partial(x,y)}{\partial(u,v)} = \sqrt{1-\chi^2}$$

maps the ellipse onto a unit circle in the uv plane, thus

$$J = 4\pi \int_{-1}^{1} du \int_{-\sqrt{1-u^2}}^{\sqrt{1-u^2}} dv \frac{g(x,y)}{\sqrt{1-u^2-v^2}}.$$

Hence a final transformation to polar coordinates (s,ξ) gives

$$J = 4\pi \int_0^1 ds \int_0^{2\pi} d\xi \frac{s}{\sqrt{1-s^2}} g(x,y),$$

with

$$\begin{aligned} x &= \tfrac{1}{2}s[(\sqrt{1+\chi}+\sqrt{1-\chi})\cos\xi \\ &\quad +(\sqrt{1+\chi}-\sqrt{1-\chi})\sin\xi] \\ y &= \tfrac{1}{2}s[(\sqrt{1+\chi}-\sqrt{1-\chi})\cos\xi \\ &\quad +(\sqrt{1+\chi}+\sqrt{1-\chi})\sin\xi]. \end{aligned}$$

So, for instance,

$$\int \delta(\boldsymbol{n}_1 \cdot \boldsymbol{n}_2 - \chi)\, d\Omega_1 d\Omega_2 = 8\pi^2$$

and

$$\int \cos\theta_1 \cos\theta_2 \delta(\boldsymbol{n}_1 \cdot \boldsymbol{n}_2 - \chi)\, d\Omega_1 d\Omega_2 = \frac{8\pi^2\chi}{3}.$$

[1] R. Lipowsky, Nature **349**, 475 (1991).

[2] F. David, in *Statistical Mechanics of Membranes and Surfaces*, edited by D. Nelson, T. Piran, and S. Weinberg (World Scientific Publishing Co. Pte. Ltd., Singapore, 1989).

[3] L. Peliti, *Fluctuations of Membranes*, Report cond-mat/9501076 (unpublished).

[4] F. C. MacKintosh and T. C. Lubensky, Phys. Rev. Lett. **67**, 1169 (1991).

[5] D. R. Nelson and B. I. Halperin, Phys. Rev. B **19**, 2457 (1979).

[6] R. M. L. Evans, J. Phys. (France) II **5**, 507 (1995).

[7] W. Helfrich, J. Phys. (Paris) **47**, 321 (1986).

[8] E. A. Abbott, *Flatland: A Romance of Many Dimensions* (Dover, New York, 1952).

[9] D. E. Rutherford, *Vector Methods* (Oliver & Boyd Ltd., London, 1959).

[10] Jeffrey R. Weeks, *The Shape of Space* (Marcel Dekker, New York, 1985).

[11] J. Park, T. C. Lubensky, and F. C. MacKintosh, Europhys. Lett. **20**, 279 (1992).

[12] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics: Non-Relativistic Theory* (Oxford Pergamon, New York, 1958).

[13] A. A. Abrikosov, Zh. Eksp. Teor. Fiz. **32**, 1442 (1957) [Sov. Phys. JETP **5**, 1174 (1957)].

[14] S. M. Roy and Virenda Singh, Phys. Rev. Lett. **51**, 2069 (1983).

[15] J. A. O'Neill and M. A. Moore, Phys. Rev. B **48**, 374 (1993).

[16] W. Cai, T. Lubensky, P. Nelson, and T. Powers, J. Phys. (France) II **4**, 931 (1994).

[17] See, for instance, G. J. Ruggeri and D. J. Thouless, J. Phys. F **6**, 2063 (1976).

[18] See, for instance, S. K. Ma, *Modern Theory of Critical Phenomena* (W. A. Benjamin, Inc., New York, 1976).

[19] G. Arfken, *Mathematical Methods for Physicists*, 3rd ed. (Academic Press Ltd., New York, 1985).