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Investigation on the ground states of a model thin-film superconductor on a sphere

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Abstract. We consider the problem of finding the ground state of a model type-II superconductor on the two-dimensional surface of a sphere, penetrated by N vortices. Numerical work shows the ground states to consist of a triangular network of the vortices with twelve five-coordinated centres. Values of N are found with particularly low-energy ground states, due to structures of high symmetry. The large-N limit is treated within elasticity theory to compare with the triangular vortex lattice that forms the ground state on an infinite flat plane. Together with numerical work this demonstrates that the thermodynamic limit $N \to \infty$ of the spherical system remains different from the flat plane due to the presence of twelve disclination defects.

1. Introduction

The problem of constructing an optimum lattice-like structure over a curved surface has become an area of interest in diverse contexts within condensed matter physics. Some examples are in work on flexible tethered membranes, Fullerene molecules, the Thomson problem of electrons on a spherical surface and in models of two-dimensional systems using a spherical geometry to study both the quantum hall effect (QHE) and thin-film superconductors.

The well known Fullerene molecules demonstrate how a low-energy structure can be formed by folding a hexagonal lattice of carbon atoms (as is found in graphite) onto a closed surface, as long as twelve five-membered rings (pentagons) are present—a simple consequence of Euler's theorem. These pentagons are essentially disclination defects in the hexagonal lattice. The first Fullerene molecule discovered was C_{60} in which each of the sixty atoms holds an identical symmetry position within the structure of the molecule, so that the atoms reside on the surface of a sphere [1]. This is a special case and as the number of carbon atoms increases in these molecules the shape may distort from a sphere to reduce the strain from the ideal hexagonal lattice over large areas. The interaction between the energy cost of bending the surface of the molecule and the strain energy within the molecule due to the disclination defects is of central importance in the question of the stability of different structures [2–4].

The same considerations are important in the behaviour of membranes with internal crystalline order and the ability to buckle out of the two-dimensional plane. A disclination defect may lower its energy by buckling. If this reduces the total energy of the defect such that it diverges at most logarithmically with the system size, then this raises the possibility of a buckling transition as defects begin to proliferate at some finite temperature [5].

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Alternatively, if we consider a closed membrane, such as a vesicle made from surfactant bilayers, then the interaction of the internal orientational order with the physical curvature may alter the shape [6], or even the topology [7] of the membrane.

Some important and well studied models involve these problems but with the curvature of the system fixed. One instance is Thomson's problem of trying to find the lowest energy configuration for N electrons that are constrained to lie on the surface of a sphere. Although the problem was first proposed in the rather dated context of classical models of the atom [8], it has been extensively studied recently. This is partly because of the general relevance to any physical system of this geometry, but also for its interest as an unsolved problem, providing a testing ground for various numerical optimization methods [9–13].

A different model where a two-dimensional system is restricted to a spherical surface has been studied both in the context of the QHE and in numerical studies on thin-film superconductors. In this model, a magnetic field perpendicular to the surface is imposed by placing a Dirac monopole at the centre of the sphere. The possible electronic states on the surface of the sphere split into Landau levels under the influence of the magnetic field, in analogy with the problem on a flat plane. The reason the model was put on a sphere by Haldane was to allow 'the construction of homogeneous states' with only a finite number of electrons [14]. Recent Monte Carlo simulations of 2D superconductors have been performed with a similar model to Haldane's with a superconducting wavefunction in the lowest Landau level on the sphere [15–17]. This wavefunction contains N zeros that correspond to vortices in the supercurrent, where N depends on the quantized strength of the monopole. The reason for using this model is again to enable translational invariance which is not possible in a finite system on a flat plane.

The Monte Carlo simulations on a sphere have led us to consider in detail the ground states of this model. While the problem of finding the ground state of an infinite type-II superconductor penetrated by vortices was long ago solved and found to be the triangular vortex lattice [18], such a lattice cannot form on a sphere without the presence of twelve vortices with only five nearest neighbours. These twelve vortices are the centres of disclination defects. By considering the strains from the perfect triangular lattice, caused by the disclination defects, within elasticity theory, we have approximated the ground-state energy in the large-N limit using similar methods used in theoretical work on membranes and Fullerene molecules. We have also found numerically the ground states with finite N, using symmetry considerations to reach large system sizes. We find values of N that give particularly low energies and this is explained. By extrapolating our numerical results to large N we find a finite energy cost per vortex on the sphere compared to the infinite plane ground state that is consistent with our results from elasticity theory.

2. Formulation

Our model thin-film superconductor consists of a spherical shell of superconducting material, thickness d, radius R and a monopole at the centre of the sphere that produces an integer multiple of flux quanta through the spherical surface. We ignore spatial fluctuations in the magnetic flux density, B, at the surface; the effective penetration depth for supercurrents in thin films becomes arbitrarily large as d is reduced. We choose a cylindrically symmetric gauge consistent with this field with $\boldsymbol{A} \equiv (A_r, A_\theta, A_\phi) = (0, 0, BR\tan\theta/2)$. We measure lengths in the units $l_m = (\Phi_0/2\pi B)^{1/2}$ which if there are N quanta of flux gives $R = (N/2)^{1/2}$. If we may describe the properties of the superconductor by a complex order

parameter $\psi(\theta,\phi)$, then the Ginzburg–Landau free-energy Hamiltonian will be given by

$$\mathcal{H}[\psi] = \int \mathrm{d}^3 r \left[\alpha(T)|\psi|^2 + \frac{\beta}{2}|\psi|^4 + \frac{1}{2m}\psi^* D^2 \psi \right] \tag{1}$$

where $D^2 = \boldsymbol{D}^* \cdot \boldsymbol{D}$ and $\boldsymbol{D} = -\mathrm{i}\bar{h}\boldsymbol{\nabla} - 2e\boldsymbol{A}$. We diagonalize the operator D^2 by expanding ψ in a basis of eigenfunctions of D^2 which form degenerate Landau levels. The degenerate set with the lowest eigenvalue may be completed by the orthonormal functions [19]

$$\psi_m(\theta,\phi) = h_m \mathrm{e}^{\mathrm{i}m\phi} \sin^m(\theta/2)\cos^{N-m}(\theta/2) \tag{2}$$

with $m = 0, N$ and $h_m = [(N+1)!/4\pi R^2 m!(N-m)!]^{1/2}$. This is the lowest Landau level (LLL) and over a large range of fields and temperatures it is a good approximation to restrict ψ to the LLL, $\psi(\theta,\phi) = Q\sum v_m \psi_m(\theta,\phi)$. We set $Q = (\Phi_0 k_\mathrm{B} T/\beta \mathrm{d}B)^{1/4}$. With this restriction we can write the Hamiltonian in terms of the basis coefficients, which for $\alpha_T < 0$ is given by

$$\begin{aligned}\mathcal{H}(\alpha_T, \{u_m\}) &\equiv k_\mathrm{B} T \alpha_T^2 \mathcal{F}(\{u_m\}) \\ &= k_\mathrm{B} T \alpha_T^2 \left[-\sum_{m=0}^{N} u_m u_m^* + \sum_{p,q,r,s=0}^{N} w_{p+q,q,r} u_p u_q u_r^* u_s^* \delta_{p+q,r+s} \right]\end{aligned} \tag{3}$$

where $w_{p+q,q,r}$ is given in [15], $\alpha_T = \mathrm{d}Q^2(\alpha(T) + eB\bar{h}/m)/k_\mathrm{B}T$ is the reduced temperature variable and we have scaled the coefficients as $v_m = u_m|\alpha_T|^{1/2}$. The quartic term in equation (3) can be rewritten to give [16]

$$\mathcal{F}(\{u_m\}) = \left[-\sum_{m=0}^{N} |u_m|^2 + \frac{1}{2N}\sum_{p=0}^{2N} |U_p|^2 \right] \tag{4}$$

where $U_p = 2\pi N \sum_{q=0}^{N} B^{1/2}(2N - p + 1, p + 1) h_q h_{p-q} \Theta(p-q)\Theta(N+q-p) u_q u_{p-q}$, $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$ is the beta function and $\Theta(q)$ is the Heaviside step function.

The vortices in this system correspond to the zeros in $\psi(\theta,\phi)$. The phase of the order parameter changes by 2π when a path is followed that encircles any zero once. This becomes clear if we make the projection

$$\zeta = \tan(\theta/2)\mathrm{e}^{\mathrm{i}\phi}. \tag{5}$$

This gives the form $\psi = \cos^N(\theta/2)\sum_{m=0}^{N} a_m \zeta^m \equiv \cos^N(\theta/2) f_N(\zeta)$. Therefore $f_N(\zeta)$ is a holomorphic function of ζ with N simple zeros in the complex-ζ plane. It can always be written in the alternative product form $f_N(\zeta) = C\prod_{i=1}^{N}(\zeta - \zeta_i)$. C is an overall complex amplitude and $\{\zeta_i\}$ are the vortex positions in the projection of equation (5). The function $\psi(\theta,\phi)$ is equally well described by the set $\{u_m\}$ or the set $\{C, \zeta_i\}$. There is no simple relation between the two, although numerical routines may be used to find the positions of the zeros for a given set of basis coefficients. Despite this lack of a simple relation from the basis coefficients to coordinates on the sphere, there are still some spatial transformations one can make using the $\{u_m\}$ formalism. For instance, rotation about the z-axis by an angle γ may be performed by the transformation $u_m \to u_m \mathrm{e}^{\mathrm{i}m\gamma}$. Reflection in the x–z plane results in $u_m \to u_m^*$. Rotation by π about the x-axis occurs under the change $u_m \to u_{N-m}$.

We are interested in the ground states of $\mathcal{F}(\{u_m\})$. We write the Hamiltonian as

$$\mathcal{F} = -\Delta + \frac{\beta_\mathrm{A}}{2N}\Delta^2 \tag{6}$$

where $\Delta = \sum u_m u_m^*$ and $\beta_\mathrm{A} = \langle|\psi_0|^4\rangle/\langle|\psi_0|^2\rangle^2 = \sum|U_p|^2/\Delta^2$ is the Abrikosov factor. This is minimized by $\Delta = -N/\beta_\mathrm{A}$ to give $\mathcal{F}_\mathrm{min} \equiv -NE_0 = -N/2\beta_\mathrm{A}$, so minimizing $\mathcal{F}$

is equivalent to minimizing $\beta_{\mathrm{A}}(\{u_m\})$. The correct Δ is then given by a scale factor on the basis coefficients that does not alter β_{A}.

The ground state of the LLL vortex system on an infinite plane is well known to be the triangular lattice [18] which has $\beta_{\mathrm{A}} = \beta_{\mathrm{A},0} \simeq 1.1596$. With periodic boundary conditions, this is also the ground state on the finite systems used in other simulations [20–22]. However, a perfect triangular lattice cannot form on a spherical surface. The closest configuration the vortices can make to an ideal lattice must contain twelve 'disclinations', i.e. twelve vortices that only have five nearest neighbours. In section 4 we give our results for directly minimizing $\mathcal{F}(\{u_m\})$ using a simple numerical method, but first we describe in section 3 calculations using elasticity theory to give the finite energy cost that the spherical system will have as $N \to \infty$ due to the twelve disclinations.

3. Elasticity theory

For a lattice in a two-dimensional plane, the elastic energy cost of deformations from the perfect ground-state lattice is given in the harmonic approximation by

$$F_{\mathrm{el}} = \tfrac{1}{2} \int \mathrm{d}^2 r \left(2\mu u_{ij}^2 + \lambda u_{kk}^2\right) \tag{7}$$

where $u_{ij}(\boldsymbol{r}) = \frac{1}{2}(\partial_i u_j(\boldsymbol{r}) + \partial_j u_i(\boldsymbol{r}))$ is the elastic strain matrix. The displacement $\boldsymbol{u}(\boldsymbol{r}) = (u_x, u_y)$ represents the deformation of the lattice from the point $\boldsymbol{r}$ to the point $\boldsymbol{r} + \boldsymbol{u}$. The elastic constants μ and λ are related to the shear and bulk moduli by $c_{\mathrm{shear}} = \mu$ and $c_{\mathrm{bulk}} = \mu + \lambda$. For the LLL ground state the bulk modulus is infinite; the vortex system is incompressible so $u_{kk} = 0$. The shear modulus is given by [23]

$$\mu = 0.48 \times \frac{1}{2}\mu_0 H_{c2}^2 \frac{(1 - H/H_{c2})^2 d}{2\kappa^2 \beta_{\mathrm{A}}^2} \,. \tag{8}$$

The GL parameter κ is the ratio of magnetic and superconducting correlation lengths, which diverges when we neglect the magnetic screening of supercurrents. In our approximation we can write the shear modulus as $\mu = 0.48 k_{\mathrm{B}} T \alpha_T^2 / 4\pi\beta_{\mathrm{A}}^2 l_m^2 = 0.0659 E_0 / l_m^2$ (this is written in terms of the energy per vortex of the ideal triangular lattice on the infinite flat plane, $-E_0$).

From the elastic energy in equation (7) Hooke's law may be derived by minimizing F_{el} to give $\partial_i \sigma_{ij} = 0$ for the stress tensor

$$\sigma_{ij} = 2\mu u_{ij} + \lambda u_{kk} \delta_{ij} \,. \tag{9}$$

The zero-divergence condition allows the reformulation of the problem in terms of the Airy stress function [24] $\sigma_{ij} = \epsilon_{ik}\epsilon_{jl}\partial_k \partial_l \chi$. (This is analogous to the vector potential that ensures zero divergence of magnetic fields.)

In the presence of topological defects, such as the disclinations we are considering, the displacement field $\boldsymbol{u}(\boldsymbol{r})$ is multi-valued. A disclination is defined by the change in bond angle $\vartheta = \frac{1}{2}\epsilon_{ij}\partial_i u_j$ as a closed loop is followed. Encircling a five-fold disclination in a triangular lattice will increase ϑ by $2\pi/6$. This results in the non-commutativity of the derivatives of ϑ at the centre of the disclination. Writing the strain field in terms of the Airy stress function results in the biharmonic equation that contains all of 2D elasticity theory [5]:

$$\frac{1}{K_0} \nabla^4 \chi = s(\boldsymbol{r}) \,. \tag{10}$$

The density of disclinations is $s(\boldsymbol{r}) = \sum_\alpha s_\alpha \delta(\boldsymbol{r} - \boldsymbol{r}_\alpha)$ where α labels each defect and $s_\alpha = 2\pi/6$ for a five-fold disclination. In equation (10), K_0 is the 2D Young's modulus, which in the LLL is

$$K_0 = \frac{4\mu(\mu+\lambda)}{2\mu+\lambda} = 4\mu = 0.264 E_0/l_m^2 . \tag{11}$$

Of course, our problem is not on a flat plane but on a sphere, so we must take into account the bending of the system out of the plane. In the large-N limit the surface will be flat locally compared to lattice spacings. Over a small region, we may approximate the sphere as a plane with some small perpendicular deflection, $f(\boldsymbol{r})$. For our purposes we neglect the bending energy which will tend to a constant—independent on the system size—when integrated over the whole sphere. However, we will need to write the strain matrix as $u_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i + \partial_i f \partial_j f)$. This alters the biharmonic equation by adding an extra term, $\det(\partial_i \partial_j f) \simeq K$, the Gaussian curvature to equation (10):

$$\frac{1}{K_0}\nabla^4 \chi = s(\boldsymbol{r}) - K(\boldsymbol{r}) . \tag{12}$$

For a sphere the curvature is constant, $K = 1/R^2$. We write χ as the superposition of twelve contributions corresponding to each disclination, $\chi(\boldsymbol{r}) = \sum_{\alpha=1}^{12} \chi_\alpha(\boldsymbol{r})$. The solution to (12) is found in the appendix. The elastic energy from equation (7) can be written in terms of the Airy stress function as in equation (A6). We have calculated the energy cost for these twelve disclinations for different configurations. For any configuration the total energy scales with the surface area of the sphere, so there is a finite energy cost per vortex in the limit $N \to \infty$. The minimum energy is found with the disclinations at the corners of an icosahedron. In this case we find an energy cost per vortex of

$$\delta E_{\rm el} = 0.0236 K_0 R^2/N = 0.0031 E_0 . \tag{13}$$

In section 4 we will compare $\delta E_{\rm el}$ with the energy δE obtained by direct minimization of $\mathcal{F}(\{u_m\})$ for finite N.

4. Numerical results

We have used a simple quasi-Newton algorithm to find configurations $\{u_n\}$ that minimize the Abrikosov ratio $\beta_{\rm A}(\{u_n\})$; this is equivalent to finding the minimum energy of the system. Clearly there are some transformations of $\{u_n\}$ under which $\beta_{\rm A}$ is invariant. The energy of the system remains unchanged after a global phase change in the order parameter, or after a rotation of the whole system about some axis. These freedoms can be fixed by restrictions on the coefficients [15]. Our results up to $N = 200$ are shown in figure 1. The presence of 'magic numbers', for which the ground state has a lower energy than nearby values, is clearly seen at $N = 12$, 32, 72, 132 and 192. To some extent we can explain the magic numbers from the expected symmetry of the most stable ground states.

By finding the zeros of the ground states, we can look at the vortex configurations. As might be expected they make up a triangular network, but with twelve five-coordinated centres. The magic number states display icosahedral symmetry with the disclinations corresponding to the corners of the icosahedron, as in figure 2. In fact, the structures appear to be projections onto the sphere of icosadeltahedra, which are polyhedra with identical equilateral triangular faces and icosahedral symmetry [25]. These may be constructed by considering the number of triangular lattice vectors between neighbouring five-fold centres, labelled by the indices (h, k).

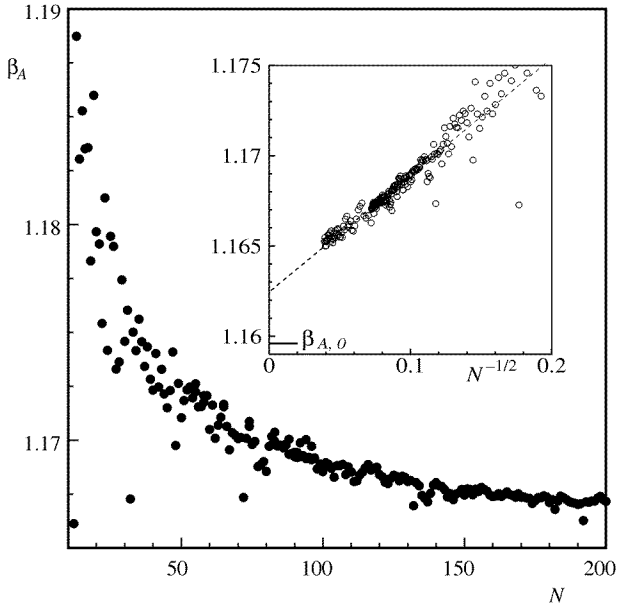

Figure 1. The minimum values of the Abrikosov ratio β_A for different system sizes. Note the low values for $N = 12, 32, 72, 132$ and 192. The inset shows the values for large N plotted against $N^{-1/2}$ with a fit to extrapolate to the $N \to \infty$ limit. The value for an infinite flat plane, $\beta_{A,0}$, is shown for comparison.

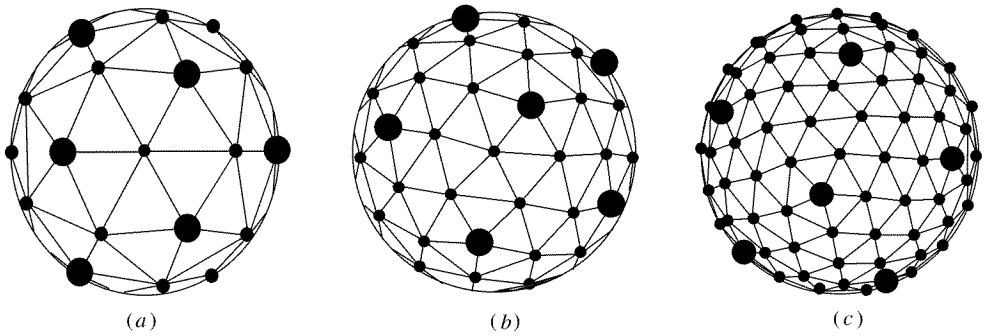

Figure 2. The numerically found ground states for three magic number cases: (*a*) $N = 32$, (*b*) $N = 72$, (*c*) $N = 132$. Only one hemisphere is shown; the full circles represent the zeros of the order parameter and the five-fold centres are represented by larger full circles, which in each case form the corners of an icosahedron.

A simple geometrical argument shows that this divides each face of the icosahedron into T triangular faces with $T = h^2 + hk + k^2$, so T may be equal to $1, 3, 4, 7, 9, 12, 13, 16, 19, \ldots$. This gives a total of $20T$ faces and $10T + 2$ vertices to the icosadeltahedra. The magic numbers we find satisfy these conditions, the only remaining question being why some possible values of N are not so low in energy, e.g. $N = 42$ or 122.

Notice that the structures for $N = 72$ and 132 possess a chirality. In fact, this will always be the case for $h \neq k$ (as long as neither is zero). This may be a factor in deciding

the lowest energy structures as the complex conjugation of the coefficients is equivalent to a reflection. If a ground state has no chirality then any reflection of the state will be equivalent to a rotation. This would require that we could write the ground state with all coefficients having the same phase. It is unlikely that this combination would be effective in minimizing the complex interactions in the quartic term of the Hamiltonian especially as the system size increases. Therefore the chirality allows a greater variety of phase differences between the coefficients. Such subtleties may explain why the ground states for some non-chiral icosahedral numbers are not particularly stable, as with $N = 42, 122$.

Remarkably, the same structures that are found when we minimize our vortex system for some magic numbers are seen in nature in the form of the shells of certain viruses [26]. In particular, the structure shown in figure 2(c) for $N = 132$ is also observed in double and single-shelled simian rotaviruses, in a left-handed configuration [27]. That these similarities exist in such different systems suggests that some general principle exists for the criterion of the most stable structure. It is possibly related to a mathematical problem that also generates these structures. This is the 'covering' problem: how may N equal overlapping circles (without gaps) cover a sphere so that the diameter of the circles is minimized [28]? The centres of these circles correspond to the vortices in our system. The alternative problem of maximizing the diameter of the circles apparently gives different solutions.

The details of the magic number states become less important as N becomes large, the limit treated in section 3 within elasticity theory. As N increases the numerical minimization becomes less trivial as there is an increasing overlap between the basis states resulting in more complex phase interference (see [29] where numerical minimization on a plane in cylindrical coordinates resulted in rather high values of β_{A}). Another possibly related problem is the growth in the number of metastable states with energies only slightly above the ground state. The numerical work on Thomson's problem has found that the number of metastable states grows exponentially with the system size [10]. We may use our knowledge of the symmetry of the most stable configurations to reduce the number of free variables by an order of magnitude. We assume the icosahedral properties of the ground state, and choose a five-coordinated vortex at $\theta = 0$. The five-fold symmetry about the z-axis is imposed by setting $u_n = 0$ for $n \neq (5m + 1)$ where m is any integer. The icosahedron also has five two-fold axes of symmetry at right angles to each five-fold axis. This two-fold rotational symmetry will arise if we set $u_n = u_{N-n}$. We have performed the same minimization routine using these constraints for $N = 10m + 2$ up to $N = 652$.

Our results for large N are shown in the inset to figure 1. The data fit well to the form $\beta_{\mathrm{A}} = A + BN^{-1/2}$ with $A \simeq 1.1624 = \beta_{\mathrm{A},0}(1 + 0.0024)$ and $B \simeq 0.0648$. As $N \to \infty$, β_{A} does not seem to converge to the infinite plane value $\beta_{\mathrm{A},0}$ (contrary to the conclusions of O'Neill and Moore from the minimizations of small system sizes [15]). This extrapolation implies a finite energy cost per vortex on the sphere in the large-N limit of

$$\delta E = 0.0024 E_0 \,. \tag{14}$$

The difference between this and the result of equation (13) from elasticity theory may be explained by the inadequacy of the harmonic approximation in this calculation. As there are large strains associated with the disclination defects, nonlinear effects will be important in determining the total energy cost. In their calculation of disclination defects on flat membranes Seung and Nelson [5] found the same mismatch between elasticity theory and numerical results, with elasticity overestimating the energy cost by a similar proportion.

Within the approximations of section 3 the correction for finite N is not predicted. Numerically the energy cost per vortex falls as $1/R$ at large N which implies a total contribution that grows proportionally to the radius.

It must be stressed that the results of this section required no great numerical effort. More sophisticated optimization methods (e.g. simulated annealing [9] and its generalizations [13]) may give greater confidence in whether or not the absolute minima have been found. More extensive work would also give results for larger N. However, our use of symmetry has allowed us to do a great deal with just a simple routine.

5. Conclusions

The original motivation of this work was for the use of the numerical ground states in Monte Carlo simulations [17]. We also wanted to investigate the differences between these ground states and the ground states on a flat plane, for which other groups have performed simulations obtaining different results. The work in this paper shows that the vortex ground states on the sphere do not approach the ground state of the infinite flat plane as $N \to \infty$. The presence of the twelve disclinations remains important however large the sphere.

This work may also be of interest in wider contexts: first, in its relation to other optimization problems of points on a sphere. Our particular system allows a use of symmetry that may not be so straightforward with position variables. This enables us to find approximate ground states at large N with quite unsophisticated numerical techniques. Our elasticity calculation may be relevant to the large-N limit of Thomson's problem, using properties of the Wigner lattice on a 2D infinite plane. This limit has been considered before, and projection of the Wigner lattice onto a spherical surface was used to estimate the extra energy on the sphere [11]. However, no consideration was taken of the required disclination defects. This paper also provides a numerical test of the accuracy of elasticity theory for curved membranes and disclination defects where the approximation of small deviations from the ideal lattice breaks down. Finally, the fact that the structures we see in the magic number ground states are the same structures seen in such a different field as virology suggests that these fascinating shapes are the result of some general optimization criteria.

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It is a pleasure to thank Mike Moore for his help and encouragement as well as Mike Evans for useful conversations.

Appendix. Disclination on a sphere

In this appendix we derive the contributions from each of the twelve disclinations to the Airy stress function $\chi(\boldsymbol{r}) = \sum_{\alpha=1}^{12} \chi_\alpha(\boldsymbol{r})$ and describe how this leads to the elastic energy cost of these disclinations. From equation (12) with $K = 1/R^2$ and $s = \frac{1}{3}\pi \sum_{\alpha=1}^{12} \delta^2(\boldsymbol{r}-\boldsymbol{r}_\alpha)$ we have

$$\frac{1}{K_0}\nabla^4\chi_\alpha = \frac{\pi}{3}\delta^2(\boldsymbol{r}-\boldsymbol{r}_\alpha) - \frac{1}{12R^2} \tag{A1}$$

where $\boldsymbol{r}-\boldsymbol{r}_\alpha = (\theta'(\alpha), \phi'(\alpha))$, and $\theta'(\alpha)$ and $\phi'(\alpha)$ are the polar and azimuthal angles with respect to the axis through the disclination. Using the symmetry about this axis, this may be integrated to give

$$\nabla^2\chi_\alpha = \frac{K_0}{12}\{\ln[1-\cos\theta'(\alpha)] + A\} \tag{A2}$$

with A a constant. For χ_α to be well defined the integral of $\nabla^2\chi_\alpha$ over the whole sphere must be zero, which means $A = 1 - \ln 2$. Integrating again leads to

$$\frac{\partial \chi_\alpha}{\partial \theta'(\alpha)} = -\frac{K_0 R^2}{12}\frac{[1-\cos\theta'(\alpha)]}{\sin\theta'(\alpha)}\ln\frac{1}{2}[1-\cos\theta'(\alpha)] \tag{A3}$$

$$\chi_\alpha = \frac{K_0 R^2}{12}\left\{-\ln 2\ln[1+\cos\theta'(\alpha)] + \int_0^{1-\cos\theta'(\alpha)}\frac{\ln x}{2-x}\,\mathrm{d}x\right\}. \tag{A4}$$

The integral in equation (A4) cannot be written as a finite number of elementary functions [30]. In deriving equations (A3) and (A4) integration constants may be chosen arbitrarily as this will not change the resulting strains (which depend on the second derivatives of χ). From equation (7) the elastic energy of the disclinations can be written as

$$F_{\mathrm{el}} = \frac{1}{2}\int \mathrm{d}^2 r\left[\frac{1+\sigma}{K_0}(\partial_i\partial_j\chi)^2 - \frac{\sigma}{K_0}(\nabla^2\chi)^2\right] \tag{A5}$$

$$= \frac{1}{2}\int \mathrm{d}^2 r\left[\frac{1}{K_0}(\nabla^2\chi)^2 - \frac{1+\sigma}{K_0}\epsilon_{ik}\epsilon_{jl}\partial_k\partial_l\left(\partial_i\chi\,\partial_j\chi\right)\right] \tag{A6}$$

with the 2D Poisson ratio $\sigma = \lambda/(2\mu+\lambda)$ equal to unity in the LLL approximation. The second term in equation (A6) only gives contributions on boundaries, and so is zero on the sphere. Therefore from equation (A2) we can find the energies of different configurations of the disclinations on the sphere.

References

[1] Kroto H W 1992 *Angew. Chem.* **31** 111
[2] Tersoff J 1992 *Phys. Rev.* B **46** 15546
[3] Witten T A and Li H 1993 *Europhys. Lett.* **23** 51
[4] Zhang Z, Davis H T, Maier R S and Kroll D M 1995 *Phys. Rev.* B **52** 5404
[5] Seung H S and Nelson D R 1988 *Phys. Rev.* A **38** 1005
[6] MacKintosh F C and Lubensky T C 1991 *Phys. Rev. Lett.* **67** 1169
Park J, Lubensky T and MacKintosh F C 1992 *Europhys. Lett.* **20** 279
[7] Evans R M L 1995 *J. Physique* **5** 507
[8] Whyte L L 1952 *Am. Math. Monthly* **59** 606
[9] Wille L T 1986 *Nature* **324** 46
[10] Erber T and Hockney G M 1991 *J. Phys. A: Math. Gen.* **24** L1369; 1995 *Phys. Rev. Lett.* **74** 1482
[11] Glasser L and Every A G 1992 *J. Phys. A: Math. Gen.* **25** 2473
[12] Edmundson J R 1993 *Acta Crystallogr.* A **49** 648
[13] Altschuler E L, Williams T J, Ratner E R, Dowla F and Wooten F 1994 *Phys. Rev. Lett.* **72** 2671
[14] Haldane F D M 1983 *Phys. Rev. Lett.* **51** 605
[15] O'Neill J A and Moore M A 1992 *Phys. Rev. Lett.* **69** 2582; 1993 *Phys. Rev.* B **48** 374
[16] Lee H H and Moore M A 1995 *Phys. Rev.* B **49** 9240
[17] Dodgson M J W and Moore M A 1996 *Phys. Rev.* B submitted
[18] Kleiner W H, Roth L M and Autler S H 1964 *Phys. Rev.* **133** 1226
[19] Roy S M and Singh V 1983 *Phys. Rev. Lett.* **51** 2069
[20] Kato Y and Nagaosa N 1993 *Phys. Rev.* B **47** 2932; 1993 *Phys. Rev.* B **48** 7383
[21] Hu J and MacDonald A H 1993 *Phys. Rev. Lett.* **71** 432; 1994 *Phys. Rev.* B **49** 15 263
[22] Sasik R and Stroud D 1993 *Phys. Rev.* B **49** 16 074
Sasik R, Stroud D and Tesanovic Z 1995 *Phys. Rev.* B **51** 3042
[23] Labusch R 1969 *Phys. Status Solidi* **32** 439
[24] Nabarro F R N 1967 *Theory of Crystal Dislocations* (Oxford: Clarendon) p 54
[25] Caspar D L D 1993 *Phil. Trans. R. Soc.* A **343** 133
[26] Caspar D L D and Klug A 1962 *Cold Spring Harbor Symp. Quant. Biol.* **27** 1
[27] Prasad B V, Wang G J, M. Clerx J P M and Chiu W 1988 *J. Mol. Biol.* **199** 269
[28] Tarnai T 1991 *J. Mol. Biol.* **218** 485
Tarnai T and Gaspar Zs 1991 *Math. Proc. Camb. Phil. Soc.* **110** 71

[29] Moshchalkov V V, Dhalle M and Bruynseraede Y 1993 *Physica* **207C** 307
[30] Gradshteyn I S and Ryzhik I M 1965 *Table of Integrals, Series, and Products* (New York: Academic) p 205