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SU(2) orientational ordering in restricted dimensions: evidence for a Berezinskiĭ-Kosterlitz-Thouless transition of topological point defects in four dimensions

Caroline S Gorham[1] **and David E Laughlin**

Department of Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, PA 15213, United States of America
[1] The author to whom any correspondence should be addressed

E-mail: caroling@cmu.edu **and** laughlin@cmu.edu

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Abstract

We employ the theory of topological phase transitions, of the Berezinskiĭ-Kosterlitz-Thouless (BKT) type, in order to investigate orientational ordering in four spatial dimensions that is characterized by a quaternion $n-$vector (i.e., $n = 4$) order parameter. Due to the dimensionality of the quaternion $n-$vector order parameter, the development of orientational order for systems that exist in four spatial dimensions must be viewed within the context of ordering in restricted dimensions. At finite temperatures, despite the development of a well-defined amplitude of the $n-$vector order parameter within separate regions, ordered systems that exist in restricted dimensions are prevented from developing global orientational phase-coherence as a consequence of misorientational fluctuations throughout the system. In four dimensions, this gas of misorientational fluctuations takes the form of spontaneously generated topological point defects that belong to the third homotopy group. These topological point defects must become topologically ordered in order to obtain a ground state of aligned order parameters at zero Kelvin; we argue that this topological transition belongs to the BKT universality class. We use standard 'Metropolis' Monte Carlo simulations to estimate the thermodynamic response functions, susceptibility and heat capacity, in the vicinity of the transition towards the ground state of perfectly aligned order parameters in our four-dimensional quaternion $n-$vector ordered model system. On lowering the temperature below a critical value, we identify a transition that results from the minimization of misorientations in the scalar phase angles throughout the system. The thermodynamic response functions obtained by Monte Carlo simulations show characteristic behavior of a topological ordering phase transition.

1. Introduction

Nearly 50 years ago, the idea of a topological phase transition driven by the condensation of topological defects was introduced and applied to understand how one can obtain orientational order in systems that exist in restricted dimensions [1, 2]. Prior to the description of this novel phase transition, the theorem of Mermin and Wagner [3] had established that systems that exhibit continuous symmetry cannot undergo spontaneous symmetry breaking in two- and one- dimensions. For ordered systems that exist in restricted dimensions, despite there being no possibility for conventional global orientational order at nonzero temperatures [3], an alternative phase transition takes place that allows for a globally phase-coherent ground state. In the case of the two-dimensional *XY* model, of complex $n-$vector (i.e, $n = 2$) order parameters, the nature of this phase transition was explained by Berezinskiĭ [1] and Kosterlitz and Thouless [2] by the introduction of topological point defects and a consideration of topological ordering.

In this work, we are motivated by the pursuit of the development of an analogous topological framework within which to understand the formation of the solid state from undercooled liquid systems. The full

orientational symmetry of the high-temperature liquid is characterized by the 3D group of proper rotations of solid spheres $G = SO(3)$. This group is a non-Abelian group, and is related to the quaternion numbers by a map from the three-sphere (S^3) onto $SO(3)$ that identifies the antipodal points of S^3. The orientational order in three-dimensional undercooled atomic liquids is therefore related [4] to a quaternion $n-$vector order parameter. We consider that the fact that all liquids are forced to undercool below the melting temperature T_M, so that a finite driving force can be established for the formation of stable clusters, is an effect of ordering in restricted dimensions for which conventional global orientational order is prevented at finite temperatures [3].

In particular, at temperatures below the melting temperature T_M, the orientational order in an undercooled liquid is characterized by the preferred orientational symmetry of atomic clustering, $H \in G$ where $G = SO(3)$. In order to apply important topological theorems [5, 6], one must ensure that the group G is a simply connected group. Therefore, the relevant orientational order parameter is determined by making use of the homomorphism [5, 6] that exists between $G = SO(3)$ and its universal covering group $SU(2)$, which is simply connected. To do this, one 'lifts' the isotropy subgroup $H \in SO(3)$ into $SU(2)$ which gives its binary representation [5–7].

The group $G = SU(2)$ is the set of unit quaternion elements, which parameterize the unit three-sphere (S^3). The relationship between $SU(2)$ and S^3 is analogous to the fact that the circle (S^1), i.e., the simplest compact Lie group, is isomorphic to the unitary group $U(1)$ such that $S^1 \cong U(1)$. The circle (S^1) is parameterized by the group of unit complex numbers in two-dimensions; this parameterization is given by Euler's formula:

$$\mathbb{C} : e^{\hat{i}\theta} = \cos\theta + \sin\theta\hat{i} = x_0 + x_1\hat{i} \quad \text{where,} \quad \hat{i}^2 = -1. \tag{1}$$

Thus, the complex number is two-dimensional and is characterized by a single scalar phase angle ($\theta \in [0, 2\pi]$):

$$\hat{\mathbf{n}} = (\cos\theta,\ \sin\theta). \tag{2}$$

By replacing the complex numbers $\mathbb{C}$ by the quaternion numbers $\mathbb{H}$, Euler's formula can be extended as a versor [8] (i.e., a quaternion of norm 1):

$$\mathbb{H} : e^{\hat{\tau}\theta} = \cos\theta + \hat{\tau}\sin\theta \quad \text{where,} \quad \hat{\tau}^2 = -1. \tag{3}$$

The condition that $\hat{\tau}^2 = -1$ means that the pure imaginary number $\hat{\tau}$ is a unit-length vector quaternion; $\hat{\tau}$ consists of three separate imaginary components: $\hat{i}^2 = \hat{j}^2 = \hat{k}^2 = -1$ and, $\hat{i}\hat{j} = \hat{k}$, $\hat{j}\hat{k} = \hat{i}$, $\hat{k}\hat{i} = \hat{j}$. The full expression of $\hat{\tau}$ is:

$$\hat{\tau} = \cos\theta_1\hat{i} + (\sin\theta_1\cos\theta_2)\hat{j} + (\sin\theta_1\sin\theta_2)\hat{k}, \tag{4}$$

where ($\theta \in [0, \pi], \theta_1 \in [0, \pi], \theta_2 \in [0,2\pi]$). Expanding the quaternion versor, it is easily seen that a quaternion number is four-dimensional:

$$\mathbb{H} : q = x_0 + x_1\hat{i} + x_2\hat{j} + x_3\hat{k}. \tag{5}$$

The quaternion orientation is defined on a three-dimensional curved manifold [9, 10] (S^3) that is embedded in 4D Euclidean space, for which:

$$x_0^2 + x_1^2 + x_2^2 + x_3^2 = R^2, \tag{6}$$

where R is the radius of the three-sphere. Thus, only three of these four coordinates are independent; these are the three scalar phase angles of $\mathbb{H}$. The quaternion then takes the form:

$$\hat{\mathbf{n}} = (\cos\theta,\ \sin\theta\cos\theta_1,\ \sin\theta\sin\theta_1\cos\theta_2,\ \sin\theta\sin\theta_1\sin\theta_2). \tag{7}$$

When considering $n-$vector ordering phenomena, e.g., by complex (i.e., $n = 2$) or quaternion (i.e., $n = 4$) order parameters, it is important to account for the effect of the geometric spatial dimensions of a sample [11, 12]. Conventional orientational ordering, i.e., by a spontaneous symmetry breaking event, is only possible within a bulk spatial dimension for a particular $n-$vector order parameter. The value of the largest geometric space dimension in which global orientational order, characterized by an $n-$vector order parameter, is no longer possible at finite temperatures is a restricted dimension [12] that has been called the lower critical dimension (D_{low}). For $n-$vector ordered systems that exist in restricted dimensions (i.e., $D \leqslant D_{\text{low}}$), at temperatures below a bulk critical transition temperature, separate ordered regions form that exhibit a well-defined amplitude of the $n-$vector order parameter [13] and that are weakly-coupled to their neighbors. The weak-coupling between nearest-neighbors permits misorientational fluctuations that prevent the development of global phase-coherence at finite temperatures.

In the case of complex $n-$vector ordered systems, that are characterized by a single phase angle parameter (θ), misorientational fluctuations in two-dimensions prevent the development of global phase-coherence [2, 11]. Thus, for complex $n-$vector ordered systems, $D_{\text{low}} = 2$. Nevertheless, a transition to a more ordered state is evident as the temperature of a 2D complex $n-$vector ordered system is lowered below a critical value. The nature of this novel phase transition was explained by the discretization of these misorientational

fluctuations as topological point defects. Below some critical temperature, these point defects form closely bound pairs and permit a phase-coherent low-temperature state; above this critical temperature, the point defects are unbound [2] and destroy phase-coherence.

In the current work, we extend the concept of a lower critical dimension to systems that express a quaternion $n-$vector order parameter. In analogy with complex $n-$vector ordered systems, misorientational fluctuations of the set of three scalar phase angles of a quaternion $n-$vector order parameter prevent the development of global orientational order at finite temperatures in four-dimensions. Thus, $D_{\text{low}} = 4$ in the case of quaternion $n-$vector ordered systems.

As has been shown in the case of two-dimensional XY systems [2], it is convenient to discretize the misorientational fluctuations that develop in restricted dimensions as topological defect elements [14, 15] that are spontaneously generated at temperatures just below the bulk critical transition temperature. In particular, the topological defect elements that are available to an $n-$vector ordered system, which exhibits a ground state manifold $\mathcal{M} = S^m$ where $m = n - 1$, are [14, 15]:

$$\pi_r(S^m) = 0 \text{ for, } r < m \tag{8}$$

$$\pi_m(S^m) = \mathbb{Z}. \tag{9}$$

That is, the only kind of non-trivial topological defect that is available to the n-vector ordered system belongs to the homotopy group $\pi_m(S^m) = \mathbb{Z}$ where $\mathbb{Z} = 0, \pm 1, \pm 2, \ldots$ is a lattice of integers that gives the topological number of the defect. Such topological defect elements exist as point defects [15] in the lower critical dimension $D_{\text{low}} = n$. This general feature will be applied to the cases of complex and quaternion $n-$vector ordering in the following sections.

In the case of complex $n-$vector orientational ordering in two-dimensions ($D_{\text{low}} = 2$), the relevant topological point defects that prevent global orientational ordering at finite temperatures belong to the fundamental homotopy group [14] ($\pi_1(\mathcal{M} = S^1)$). Similarly, in the case of quaternion $n-$vector orientational ordering, the relevant topological point defects belong to the third homotopy group ($\pi_3(\mathcal{M} = S^3)$). In restricted dimensions, a Berezinskiĭ-Kosterlitz-Thouless (BKT) type topological transition [1, 2] driven by the ordering of these topologically stable point defect elements is required in order to explain how an orientationally phase-coherent low-temperature state can be obtained at low-temperatures.

In this paper, we study the orientational ordering of a quaternion $n-$vector ordered system that exists in the lower critical dimension $D_{\text{low}} = 4$. Firstly, in section 2, we review the prototypical Berezinskiĭ-Kosterlitz-Thouless topological ordering transition that allows for the development of a low-temperature globally phase-coherent state of complex $n-$vector order in two-dimensions. In section 3, we consider a natural extension of this topological transition to quaternion $n-$vector ordered systems that exist in four-dimensions. In section 4, we present Monte Carlo (MC) simulations that have been performed to study the thermodynamic response functions of this four-dimensional system in the vicinity of the topological ordering transition.

2. $U(1)$ systems

2.1. Hamiltonian potential energy and 2D BKT transition

In the case of 2D systems that possess $U(1)$ symmetry at high-temperatures, a finite driving force for complex $n-$vector orientational ordering develops below a bulk critical transition temperature T_C. Just below T_C, complex $n-$vector order develops within separate regions/islands (that are weakly-linked to their nearest-neighbors) rather than across the entire system [13]. These regions/islands are characterized by separate complex $n-$vector order parameters that act as $O(2)$ rotors [16, 17], whose orientation has the form of equation (2). Despite the development of an amplitude of the complex $n-$vector order parameter within each island, misorientational fluctuations of the single scalar phase angle parameter (θ) prevent the development of global phase-coherence at finite temperatures.

Although a conventional ordering phase transition is excluded in this scenario, in order to explain how an orientationally phase-coherent low-temperature state can be obtained, Berezinskiĭ [1] and Kosterlitz and Thouless [2] introduced the concept of topological point defect excitations (metastable states). The phase-destabilizing misorientational fluctuations are naturally discretized as point defects, that undergo a topological ordering event at a finite temperature $T_{\text{BKT}} < T_C$. At high-temperatures, these point defects are spontaneously generated; at temperatures below T_{BKT}, point defects and anti-point defects form low-energy bound pairs that allow for the existence of a phase-coherent low-temperature state [1, 2].

In order to determine the critical transition temperature (T_{BKT}), one must consider the potential energy due to coupling between nearest-neighbor order parameters. The potential energy is:

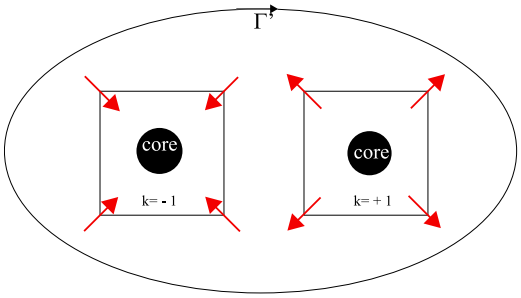

Figure 1. A loop Γ′ enclosing a pair of point defect cores with equal and opposite winding number will be topologically equivalent to the defect-free state [14].

$$V = -E_J \sum_{\langle ij \rangle} \hat{\mathbf{n}}_i \cdot \hat{\mathbf{n}}_j, \tag{10}$$

where $\hat{\mathbf{n}}_j$ is the complex $n-$vector order parameter located at site j, E_J is the Josephson interaction energy between nearest-neighbor rotors [18], and the sum is taken over the nearest-neighbors $\langle ij \rangle$. To solve equation (10), one must consider that the dot product of imaginary numbers (say, **A** and **B**) generalizes to [19]:

$$\mathbf{A} \cdot \mathbf{B} = \sum A_i B_i^{\dagger} \tag{11}$$

where the † over B_i represents the complex conjugate. Making use of the fact that $\hat{i}^2 = -1$, and using a standard cosine angle difference identity, the potential energy can be written in its traditional form:

$$V = -E_J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j). \tag{12}$$

A spin-wave approximation can be applied to equation (12), by assuming that the orientation of the rotors varies smoothly from site to site within the array [18, 20, 21].

In order to apply the spin-wave approximation, one expands the cosine in the Hamiltonian by the first two terms in its Taylor series expansion, i.e., $1 - \frac{1}{2}(\theta_i - \theta_j)^2$. Taking the sum over nearest-neighbors corresponds to the discrete Laplace operator, which can be expressed in terms of partial derivatives: $\theta_i - \theta_j = \partial_x \theta$, for sites i and j which are nearest-neighbors [22]. This leads to a continuum expression of potential energy [2, 21]:

$$V_{\text{gradient}} = \frac{E_J}{2} \int d^2\mathbf{r} (\nabla \theta(\mathbf{r}))^2, \tag{13}$$

where V_{gradient} is the gradient potential energy that is related to misorientations in θ throughout the system, from the ground state of perfectly aligned rotors. The critical properties of this system have been shown to be dominated by the long-range effects associated with misorientational fluctuations [2, 21].

Although the ground state of this system is unstable against low-energy spin-wave excitations [1, 3], one may characterize a topological ordering transition by the introduction of topological point defects [2] in the orientational order parameter field. In two-dimensional arrays of complex $n-$vector order parameters, these topological excitations arise naturally around elementary closed circuits of nearest-neighbors [14, 23] (i.e., elementary plaquettes). Non-trivial point defect configurations are defined around a closed path (Γ) of nearest-neighbors, where the sum of the relative scalar phase angles ($\theta_{ij} = \theta_i - \theta_j$) around the circuit is an integer multiple of 2π. The strength of the topological defect, also known as its winding number, can be any arbitrary integer $k = 0, \pm 1, \pm 2, \ldots$. Topological defect elements are spontaneously generated below T_C (the group $G = U(1)$ is broken locally at T_C), and are topologically stable against decay [14].

At high-temperatures, topological point defects are stabilized as isolated entities (unbound) due to the large entropy that is associated with their configurational degeneracy (related to the possible placement of the point defect core within the system [2, 24]). On the other hand, bound pairs of point defects with equal and opposite topological winding number (i.e., sum-0) are energetically preferred below a critical temperature [25]. This is a consequence of the Abelian nature of point defects, such that a path Γ' enclosing two single point defects with winding numbers k_1 and k_2 is homotopic to the two paths enclosing the point defects individually [14] (figure 1). The critical BKT transition temperature, that marks the binding of topological point defects into low-energy (sum-0) pairs, is determined by considering the competition between the entropy and energy of an isolated point defect within the context of the Helmholtz free energy: $F = V_{\text{defect}} - \text{TS}_{\text{config}}$.

The gradient potential energy associated with the slow spatial variation of the scalar phase angle variable (θ) far from an isolated point defect core [2, 14] is:

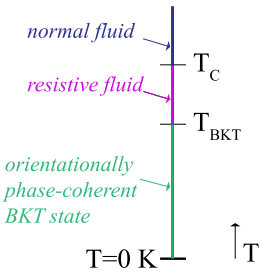

Figure 2. In two-dimensions, as the temperature is lowered below the bulk critical transition temperature T_C, a normal fluid transitions to a resistive fluid that presents a gas of misorientational fluctuations in the form of spontaneously generated point defects. An orientationally phase-coherent state is achieved by a defect-driven topological ordering event at a subsequently lower temperature T_{BKT}.

$$V_{\mathrm{defect}} = \pi E_{\mathrm{J}} \ln\left(\frac{L}{a}\right), \tag{14}$$

where a is the radius of the point defect core and L is the system size. The energy of the point defect increases logarithmically with the size of the system because, at large distances from the defect core, the gradient potential energy produced is inversely proportional to the distance [2, 14]. As a consequence, the probability of isolated topological point defects appearing in large systems will be almost nonexistent at low-temperatures [2, 14, 25].

In two-dimensions, an isolated point defect core can be located within any elementary closed circuit of nearest-neighbors; therefore, the configurational degeneracy [2, 24] may be approximated as $(L/a)^2$. The entropy associated with the configurational degeneracy is $S_{\mathrm{config}} = 2k_{\mathrm{B}} \ln\left(\frac{L}{a}\right)$, where k_{B} is the Boltzmann constant. The total Helmholtz free energy of an isolated point defect (of strength $|k| = 1$) is therefore:

$$F = \ln\left(\frac{L}{a}\right)(\pi E_{\mathrm{J}} - 2k_{\mathrm{B}}T), \tag{15}$$

where the terms in $\ln\left(\frac{L}{a}\right)$ have been collected. Since both energy and entropy depend on the system size logarithmically, the energy term will dominate the free energy at low temperatures [2]. For temperatures below $T_{\mathrm{BKT}} = \frac{\pi}{2k_{\mathrm{B}}} E_{\mathrm{J}}$, point defects should only occur in low-energy bound pairs of opposite signs which are confined logarithmically. This topological ordering event allows for the development of a low-temperature BKT state, that is orientationally phase-coherent. The series of transitions followed on the path towards the low-temperature BKT state are summarized in figure 2.

These free energy arguments, that enable the prediction of the critical BKT transition temperature, are complemented well by straightforward topological arguments. For $n-$vector ordered systems that exist in the lower critical dimension D_{low}, at temperatures just below a bulk critical transition temperature, $\pi_m(S^m) = \mathbb{Z}$ point defects are spontaneously generated. These defects are topologically stable, and thus cannot be made to disappear with any continuous deformations of the order parameter. Such point defects, when isolated, produce energetically costly distortions in the scalar phase angle parameters (here, $\theta(\mathbf{r})$) far from their core. However, owing to the Abelian nature of the $\pi_m(S^m) = \mathbb{Z}$ homotopy groups [14], pairs of point defects with equal and opposite sign (sum-0) are possible which do not require such energetically costly distortions [14]. A sum-0 pair of point defects leads to a configuration of the order parameter far from the pair that can be continuously distorted to the uniform state [14]. It follows that these low-energy pairs of point defects, which are topologically equivalent to the uniform (defect-free) state [14], are favored at low-temperatures and represent important excitations from the orientationally phase-coherent ground state.

2.2. Response functions

In the vicinity of a Berezinskiĭ-Kosterlitz-Thouless transition, the susceptibility (χ) is predicted to diverge [12, 21] as a function of a diverging correlation length (ζ). In the two-dimensional XY model, it follows from the relationship between χ and ζ (Kosterlitz [21] 1974), that the maximum of the susceptibility is proportional to the system size as [26, 27]:

$$\chi_{\mathrm{max}} \approx L^{2-\eta}, \tag{16}$$

where η is a critical exponent of the BKT transition. This is a consequence of the fact that the correlation length ζ diverges towards a maximum value equal to the sample length (L) as the critical temperature T_{BKT} is approached from above. In the case of 2D BKT transitions, it has been established that the critical exponent η takes on the value of $1/4$ at the transition temperature [12, 21, 27, 28].

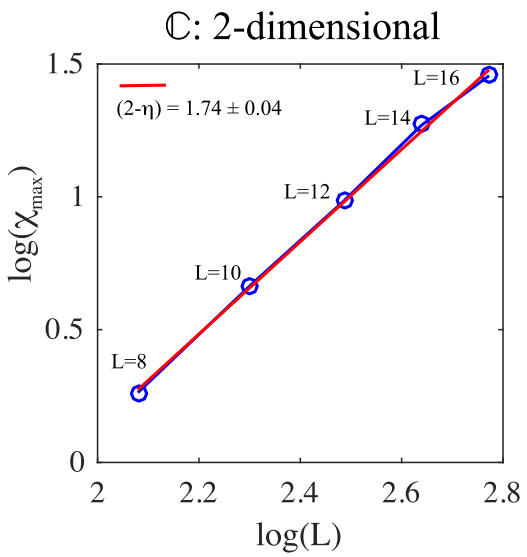

Figure 3. 2D complex $n-$vector ordered system: $\chi_{\max}$ versus system length (L) on a log-log scale [26, 27]. The slope of a straight line through the data is related to the critical exponent η in the vicinity of the BKT transition [2].

In fact, the critical exponent η depends on temperature as [12]: $\eta = \frac{k_B T}{(2\pi) E_J}$. The value of $\eta = 1/4$ allows us to recover the definition the critical BKT temperature: $T_{\mathrm{BKT}} = \frac{\pi}{2k_B} E_J$. The necessary condition for the stability of the low-temperature phase-coherent state is that $\eta(T) \leqslant 1/4$, which indicates that point defects are only excited as bound pairs [25, 28].

Using numerical Monte Carlo simulations [26, 27], one can obtain the value of the critical exponent η. In particular, the peak values of χ (i.e., $\chi_{\max}$) scale with a power of the system size L; on a logarithmic scale [26, 27], one obtains a linear fit: $\log(\chi_{\max}) = (2 - \eta)\log(L)$. We have performed Monte-Carlo simulations on two-dimensional XY systems in order to determine the critical exponent η of the 2D BKT transition; such a study has been performed previously by a number of authors [26, 27]. The peak values of the susceptibility as a function of L, for system sizes ($L \times L$) where $L = 8$,10,12,14,16, are plotted in figure 3 on a log-log scale. A linear fit to the slope of the data points gives a value of $\eta = 0.26 \pm 0.04$, which is near to the anticipated value of $\eta = 1/4$.

3. $SU(2)$ systems

As a direct higher-dimensional analogue to the 2D complex $n-$vector ordered systems, studied in section 2, a system that possesses $SU(2)$ orientational symmetry at high-temperatures and exists in four-dimensional space ($D_{\mathrm{low}} = 4$) will be unable to develop global orientational ordering (by a spontaneous symmetry breaking event) at finite temperatures. In such systems, for temperatures below a bulk critical transition temperature T_C, a finite driving force develops for a quaternion $n-$vector (i.e., $n = 4$) orientational order parameter. A four-dimensional arrangement of 4D regions (localized in space) develops, wherein each region expresses an amplitude of the orientational order parameter. These separate regions are weakly-coupled to their nearest-neighbors, and act as $O(4)$ rotors with an orientation of the form of equation (7).

In four-dimensions, despite the development of a well-defined amplitude of a quaternion $n-$vector orientational order parameter within each separate region, the system as a whole is unable to develop global orientational order as a result of misorientational fluctuations in the order parameter throughout the system. Despite the inability of the system to undergo a conventional ordering phase transition at the bulk critical transition temperature T_C, the system may still obtain a perfectly orientationally-ordered ground state by the minimization of potential energy [16]. The potential energy, due to coupling between nearest-neighbor $O(4)$ rotors, is:

$$V = -J \sum_{\langle mn \rangle} \hat{\mathbf{n}}_m \cdot \hat{\mathbf{n}}_n. \tag{17}$$

where $\hat{\mathbf{n}}_m$ is the quaternion $n-$vector order parameter located at site m, $J > 0$ is the interaction energy between nearest-neighbor order parameters, and the sum is over nearest-neighbors $\langle mn \rangle$. Making use of the fact that $\hat{i}^2 = \hat{j}^2 = \hat{k}^2 = -1$, and using a standard cosine angle difference identity, the potential energy takes the form:

$$V = -J\sum_{\langle mn\rangle}(\cos\theta_m \cos\theta_n + \sin\theta_m \sin\theta_n \times (\cos\theta_{1,m}\cos\theta_{1,n} + \sin\theta_{1,m}\sin\theta_{1,n}[\cos(\theta_{2,m} - \theta_{2,n})])). \quad (18)$$

As the temperature of the system of $O(4)$ rotors is lowered towards zero Kelvin, this potential energy function is minimized by the state of perfectly aligned rotors [16].

In this case, as a higher-dimensional analogue to the two-dimensional XY model [2, 29], an alternative form of a phase transition should occur that is topological and defect-driven. In order to understand this transition, it is instructive to discretize the misorientational fluctuations (that force the system to undercool) as spontaneously generated topological point defect excitations that belong to the third homotopy group [15], i.e., $\pi_3(S^3) = \mathbb{Z}$. With the introduction of third homotopy group point defects and anti-point defects, as topological excitations, one is able to determine the characteristics of this topological ordering transition.

To think of defect elements that belong to the homotopy group $\pi_m(S^m)$, one has to consider how many distinct ways an $m-$sphere can be wrapped around itself. In general, for each $\pi_m(S^m)$ homotopy group, there are topologically stable configurations indexed by an integer, i.e., $\pi_m(S^m) = \mathbb{Z}$. The number of times the $m-$dimensional sphere (S^m) wraps around itself is the integer topological number that defines the topological charge of the defect [14, 30, 31]. Importantly, since the group of integers $\mathbb{Z}$ is an additive group [6], the homotopy groups $\pi_m(S^m)$ are necessarily Abelian [14, 32], i.e., the rule for combining $\pi_m(S^m)$ defect elements is that their topological numbers add.

The simplest example of a $\pi_m(S^m)$ defect element belongs to the fundamental homotopy group of $\mathcal{M} = S^1$, i.e., $\pi_1(S^1) = \mathbb{Z}$, as was introduced in section 2. These topological defect elements are of crucial importance to the explanation of how a low-temperature phase-coherent state can be obtained for complex $n-$vector ordered systems that exist in two-dimensions [1, 2, 25], where they exist as point defects. In section 2, both energetic and topological arguments were made in discussing this topological ordering transition in two-dimensions. The topological arguments rely entirely on the Abelian nature of $\pi_m(S^m)$ defects, by which the possibility of the existence of sum-0 pairs of point defects may be anticipated. Such pairs of point defects lead to far-field configurations of the order parameter that can be distorted continuously to the uniform state [14]. Thus, whereas isolated point defects (which cannot be removed by any continuous distortion of the order parameter field) produce energetically costly distortions in the order parameter field, sum-0 pairs do not. It follows that these sum-0 pairs of topological point defects represent important excitations from the orientationally phase-coherent ground state.

Similarly, the core of topological defect elements of the third homotopy group of $\mathcal{M} = S^3$, i.e., $\pi_3(S^3) = \mathbb{Z}$, are points in four dimensions. Representatives of the third homotopy group are characterized by a topological number, similar to the winding number of a $\pi_1(S^1)$ defect, that measures the number of times a map of $\hat{\mathbf{n}}(\theta, \theta_1, \theta_2)$ in domain space wraps around the topological manifold $\mathcal{M} = S^3$. The topological number, which may be called B, is calculated by: (1) taking the integral of the Jacobian [33] of the map of $\hat{\mathbf{n}} \in S^3$ to $\mathcal{M}$, which counts the volume mapped out on $\mathcal{M}$, (2) dividing by $(2\pi^2)$ to arrive at the number of times each point on $\mathcal{M}$ is visited. By not taking the absolute value of the Jacobian, both positive and negative topological numbers [30] are measured. Thus, the maps from S^3 to S^3 are classified by any integer (positive or negative), i.e., $B = 0, \pm 1, \pm 2...$, and there are an infinite number of topologically distinct point defects that belong to the group $\pi_3(S^3) = \mathbb{Z}$.

At temperatures just below the bulk critical transition temperature T_C, topological point defects are free (unbound) and are spontaneously generated by pairs of opposite topological number. In the classical limit, i.e., equation (17), the concentrations of point defects with opposite signs are equal. Although there is a significant energy cost to introduce isolated point defects, due to large misorientations in the order parameter far from the defect core, these isolated excitations are stabilized at high-temperatures by configurational entropy[2]. On the other hand, for temperatures below a critical value, minimization of the potential energy (equation (17)) minimizes the Helmholtz free energy ($F = V_{\text{defect}} - \text{TS}_{\text{config}}$) and favors the perfect alignment of order parameters throughout the system. This requires that the topologically stable point defects become bound into sum-0 pairs that do not require the same energetically costly deformations that plague isolated point defects [14]. These low-energy paired configurations minimize the global uncertainty in the scalar phase angles across the system, and allow for the development of a ground state of perfect orientational order. As the temperature of the system is driven towards zero Kelvin, continuous distortions of the order parameter field can bring the two point defects that comprise a sum-0 pair together and cause them to annihilate. Thus, such paired

[2] Assuming a simple hyper-cubic lattice ($\mathbb{E}^4$), the possible positions for the placement of an isolated point defect core (located at the center of any closed hyper-volume made by nearest-neighbors) can be approximated as $(L/a)^4$ where L is the system size and a is the radius of the point defect core. The configurational entropy per point defect is then: $S_{\text{config}} = 4k_B \ln\left(\frac{L}{a}\right)$.

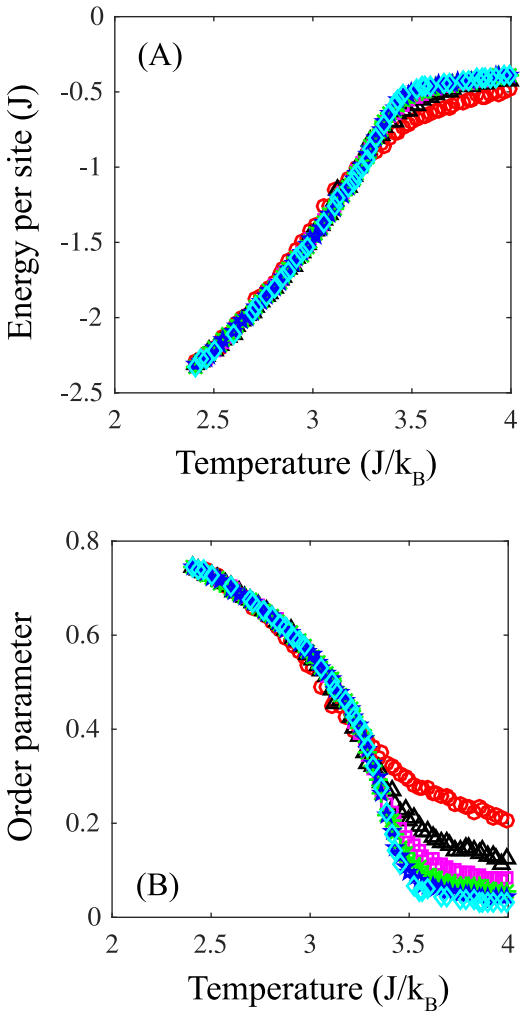

Figure 4. (A) Energy and (B) order parameter per site versus temperature for various lattice sizes ($L \times L \times L \times L$): $L = 3, 4, 5, 6, 7, 8$ ($\circ, \triangle, \square, *, \star, \Diamond$).

configurations of third homotopy group point defects represent important excitations from the orientationally-ordered ground state of four-dimensional quaternion $n-$vector ordered systems.

4. 4D Monte Carlo simulations

4.1. Methods

We use a numerical 'Metropolis' Monte Carlo (MC) algorithm to estimate thermodynamic response functions in the vicinity of the transition towards the orientationally-ordered low-temperature state of a four-dimensional system of quaternion $n-$vector order parameters (i.e., $O(4)$ rotors). The potential energy due to coupling between nearest-neighbors takes the form of equation (17). For simplicity, the $O(4)$ rotors are arranged at the sites of a simple hyper-cubic ($\mathbb{E}^4$) lattice such that each rotor has a set of eight nearest-neighbors, i.e., the kissing number [34] is eight. We make use of periodic boundary conditions, and consider system sizes $L \times L \times L \times L$ for: $L = 3,4,5,6,7,8$.

Five separate samples, initialized with different random number generators, are used to compute the physical observables for each system size L. The initial configuration of quaternion $n-$vector order parameters within the 4D array is constructed by generating a randomized distribution of scalar phase angles $(\theta, \theta_1, \theta_2)$ throughout the system. At each temperature, 1000 Monte Carlo steps are taken to achieve thermal equilibrium, and 2000 subsequent steps are used to collect the statistical data required to compute the physical observables. On each step L^4 rotors are selected in turn, and at random, and an attempt is made to change its state. The authors note that, the limited number of steps taken is a consequence of the higher dimensionality of the model which pushes the limits of our resources due to the serial nature of our code.

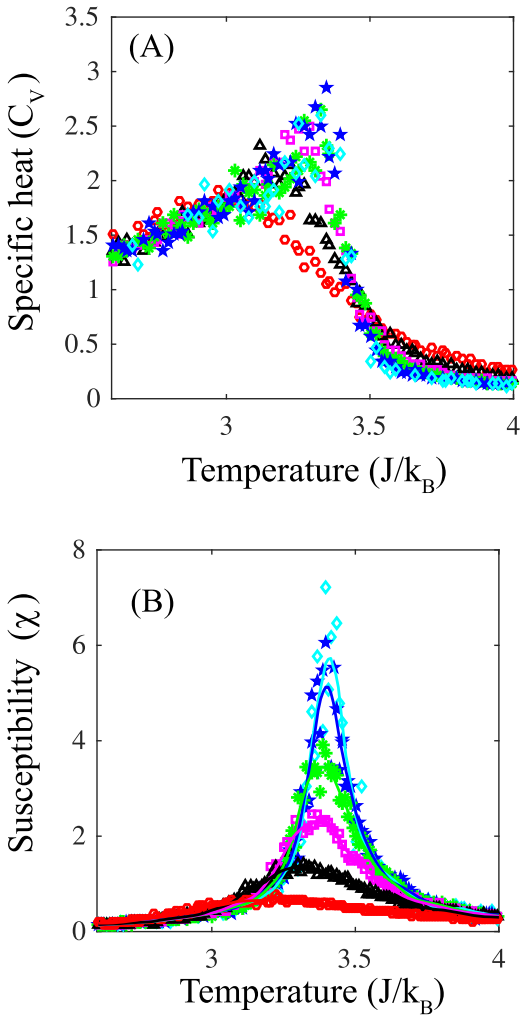

Figure 5. (A) Specific heat and (B) susceptibility versus temperature for various lattice sizes ($L \times L \times L \times L$): $L = 3, 4, 5, 6, 7, 8$ ($\circ, \triangle, \square, *, \star, \Diamond$).

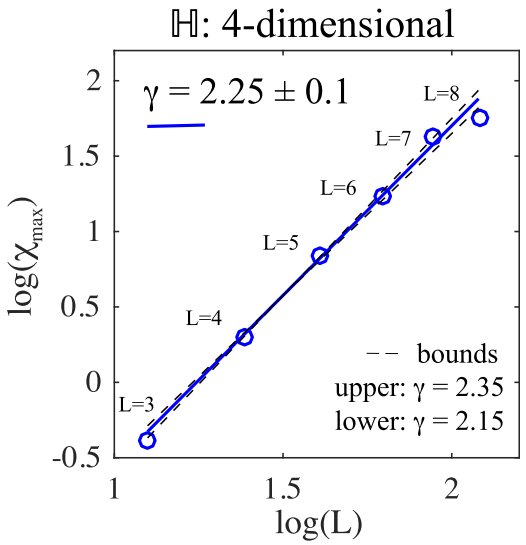

Figure 6. 4D quaternion $n-$vector ordered system: χ_{max} versus system length (L) on a log-log scale [26, 27].

As the Monte Carlo simulation proceeds, physical observables of interest are computed. The critical behavior of a topological ordering transition may be determined by considering the thermodynamic response functions: heat capacity and susceptibility [12, 21, 26, 27]. The total susceptibility of a system of N rotors is proportional to fluctuations in the order parameter:

$$\chi = \frac{1}{Nk_B T}[\langle \tilde{\hat{\mathbf{n}}}^2 \rangle - \langle \tilde{\hat{\mathbf{n}}} \rangle^2], \tag{19}$$

where $\tilde{\hat{\mathbf{n}}} = \sum_i^N \hat{\mathbf{n}}_i$, and $\hat{\mathbf{n}}_i$ is the orientational order parameter per site i. Similarly, the specific heat is proportional to energy fluctuations:

$$C_V = \frac{1}{Nk_B T^2}[\langle E^2 \rangle - \langle E \rangle^2], \tag{20}$$

where E is the total energy of the system. Figures 4(A) and (B) plot the observed energy and order parameter per site, which show evidence of a phase transition that results from the alignment of order parameters as the temperature is lowered below a critical value.

4.2. Response functions

The specific heat and susceptibility response functions are plotted versus temperature in figures 5(A) and (B), for the six lattice sizes studied. It can be seen that the peak height of the specific heat does not depend on L for large enough system sizes ($L = 6, 7, 8$), and converges to a single value. This is an indication of a topological ordering transition [27, 35]. In the case of 2D BKT transitions, the fact that the specific heat is independent of the lattice size for large enough lattices [27, 35] is well-known and this behavior has been used by many authors as an indication of the BKT transition character [27, 35].

In contrast to the specific heat, the peak value of the susceptibility does scale with system size over all length scales [26, 27]. Figure 6 plots the peak values of χ versus system size on a log-log scale; a linear fit to the data points, i.e., $\log(\chi_{\max}) = \gamma \log(L)$, can be made with a slope of $\gamma = 2.25 \pm 0.1$. This finding shows a finite scaling relationship [21, 26, 27] between the susceptibility and a diverging correlation length [21], which is another characteristic of a topological ordering transition. An analytical prediction of the value of γ requires analogous renormalization-group work to that of Kosterlitz [21] (1974).

5. Conclusions

We have detected a phase transition within a quaternion $n-$vector (i.e., $n = 4$) ordered system in four-dimensions using numerical Monte Carlo simulations. In light of the fact that the lower critical dimension for the quaternion $n-$vector ordered system is four, we have considered the transition to the low-temperature orientationally-ordered state within the context of a topological ordering phase transition of the Berezinskiĭ-Kosterlitz-Thouless (BKT) type. In order to understand the nature of this novel phase transition, we have introduced point defects that belong to the third homotopy group as topological excitations. We have provided topological arguments which show that, below a critical temperature, these topological point defects bind into low-energy pairs and thereby allow for the existence of an orientationally-ordered low-temperature state.

In order to verify the transition type, we monitored the response functions of specific heat and susceptibility for several lattice sizes using our Monte Carlo simulations. We found that the specific heat is independent of the lattice size for large enough lattices, which is indicative of a topological ordering transition. Furthermore, we found evidence of strong finite size scaling of the susceptibility with a power of the lattice size. This kind of strong scaling is known to occur in the vicinity of a BKT-type topological ordering transition. Thus, we conclude that our Monte Carlo results provide evidence that the transition to the orientationally-ordered low-temperature state of a quaternion $n-$vector ordered system in four-dimensions belongs to the Berezinskiĭ-Kosterlitz-Thouless universality class of topological ordering phase transitions.

To summarize, in the current paper, we have extended the concept of topological ordering transitions to a higher-dimensional algebra domain (i.e., quaternions). As future work, we suggest that this quaternion $n-$vector model may be applied to real systems in order to understand the topological nature of the liquid-to-solid phase transition in three-dimensions, for which undercooling below the melting temperature is necessary.

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ORCID iDs

Caroline S Gorham https://orcid.org/0000-0002-9135-1003
David E Laughlin https://orcid.org/0000-0002-9819-7897

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