Critical behavior of the helicity modulus for the classical Heisenberg model

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The critical scaling of the helicity modulus of the classical O(3) $3d$ Heisenberg ferromagnet is studied directly. Monte Carlo methods that impose either an antiperiodic boundary condition or a finite twist of definite handedness across otherwise periodic boundaries in one lattice direction are used to measure scale-dependent enthalpy variations in a simple cubic lattice at the ferromagnetic critical temperature. Finite-size scaling is then used to determine the critical exponents v_E and v_F for helicity and, by evaluating three independent hyperscaling-linked pairs of ν and α, to test hyperscaling for this model. It is observed that antiperiodic boundary conditions in particular constrain the lattice to have a nonzero topological charge, establishing a connection between topological charge and helicity in the model.

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I. INTRODUCTION

The helicity modulus (spin-wave stiffness) Υ is a direct measure of the response of an ordered, isotropic system to a suitable helical or "phase twisting field" [see Fisher, Barber, and Jasnow[1] (FBJ)]. As such, it is a quantity of great interest in studies of the critical behavior of O(n)-symmetric continuous spin systems such as O(2) superfluids (where it has been studied with Monte Carlo methods)[2–5] or the O(3) classical Heisenberg model. For example, the helicity modulus can be shown to be equal to the effective superfluid fraction in a suitably granulated model of superconductivity.[6]

There are still open questions in symmetric spin systems, in particular whether or not there is a topological element to the phase transition. A number of researchers have looked at the phase transition for O(3) spins in a three-dimensional lattice to try to determine whether or not it can fairly be characterized as an unbinding of hedgehog (chargelike) defects in the spin field, similar to the way the transition in O(2) XY models can be viewed as the unbinding of current-like defects (spin loops of opposite handedness).[7–11]

Helicity is also of interest in closely related chiral field theories;[12] the ordered phase of continuous isotropic systems is characterized by both the appearance of Goldstone (transverse) modes and an associated breakdown of the disordered phase's exponential decay of correlations in both condensed matter and field theories. However, the connection of helicity with topological charge has not been studied in the O(3) models in particular.

The critical scaling of the helicity modulus is a useful thing to study in continuous spin systems. The correlation function is extremely difficult to study directly with, e.g., Monte Carlo methods on a lattice with periodic boundary conditions because the existence of periodic images of a spin causes a significant deviation of the correlation function from its asymptotic form in precisely the asymptotic region one is hoping to fit. However, the energy response to a helical twist of the image spins a maximal distance away yields direct information about the correlation decay across the entire intervening range as it effectively constrains the system to populate the specific long-wavelength spin modes that are energetically consistent with the temperature. FBJ showed that the helicity modulus may be used to define a "phase coherence length," which has been conjectured to be the actual correlation length in the ordered phase for a variety of models [see the discussion around their equation (3.9)].

This conjecture (as is outlined below) rests upon the validity of hyperscaling (lattice dimension d dependent) relations such as $d\nu=2-\alpha$. If hyperscaling can be shown to be valid for the model, Monte Carlo measurements of the helicity modulus yield direct information about the transverse correlation function and hence increase our understanding of the structure of the ordered phase near criticality.

In addition, if we measure at least one nonhyperscaling critical exponent ratio such as β/ν while conducting such a Monte Carlo experiment, the rest of the static critical exponents for the model can be determined from (say) β and ν and the usual scaling and hyperscaling relations.

To these ends this work studies the critical behavior of helicity in the O(3) model in three lattice dimensions (the isotropic classical Heisenberg ferromagnet). The microscopic Hamiltonian corresponding to this model in the absence of a symmetry breaking external field is

$$\mathcal{H} = -J \sum_{i<j}^{\text{neighbors}} \vec{S}_i \cdot \vec{S}_j, \tag{1}$$

where the sum is over nearest-neighbor spins only. The spins are classical unit vectors in three dimensions, $\vec{S}=s_x\hat{x}+s_y\hat{y}+s_z\hat{z}$, with $+\sqrt{s_x^2+s_y^2+s_z^2}=1$. Equivalently the spins can be described by a pair of angles on a unit sphere in spherical polar coordinates.

Using the Monte Carlo methodology described in detail below, the related critical exponents of the helicity modulus v_E and v_F were computed. The exponent v_F is related in known ways to α and ν as shown in FBJ. The critical exponent ratio α/ν was directly evaluated by fitting the finite-size scaling of $E(T_c,L)$ and $C(T_c,L)$ independently from the resulting Monte Carlo data. The results of these three distinct computations were then compared and found to be in excellent agreement with each other subject to the assumption of hyperscaling. A consistent set of hyperscaling exponents α and ν and the helicity exponents v_E and v_F with reasonable error bounds were estimated as a consequence of this comparison.

While accumulating the Monte Carlo data used to measure the helicity exponents and energy moment exponents, the data required one to perform a very-high-precision finite-size scaling computation of the exponent ratio β/ν (or the critical exponents of other order-parameter moments) were also sampled and accumulated. In all cases the computations were run indefinitely in a loop that distributed independent runs (each with a unique random number seed) onto the nodes in a compute cluster until demanding relative precision targets (reliably evaluated using the standard deviation associated with independent *runs*) were reached over the entire $\log_{10}$ decade being fit.

As discussed below, the order parameter, energy, and helicity averages thus obtained at T_c for various L were *too precise* over *too large a range of* L for a traditional finite-size scaling fit to work (with a single nonanalytic algebraic term and no confluent corrections) and still produce an acceptable χ^2. In most cases (with the notable exception of the energy) an additional algebraic confluent term was required to accommodate the low-L measurements in the fit and obtain an acceptable χ^2 over the largest possible range of L. The correction term generally *improved the asymptotic character of the fit* by not requiring data that clearly fall on a confluent curve (on a log-log scale) that has not yet reached its asymptotically straight form to be fit by a straight line.

II. CRITICAL SCALING OF THE HELICITY MODULUS

The helicity modulus was introduced by FBJ in Ref. 1 by the definition

$$\Delta F(\Theta) \approx \frac{1}{2}\Upsilon_F(T)(\nabla\phi)^2, \tag{2}$$

where $\Delta F(\Theta)$ is the change in the free energy density when the periodic boundary condition on one face of an L^3 cube (for example) of $O(n)$ ferromagnetic spins is twisted by the angle Θ (as $L\to\infty$) relative to its periodic partner. For $|\Theta| \leq \pi$, this introduces a continuous Möbius twist in the spins along one axis of the periodic three-torus. $\nabla\phi=\Theta/L$ is the average gradient of the twist angle across the cube; for small Θ this corresponds to forcing, in thermal equilibrium, the excitation of a long-wavelength ($\lambda \gg L$) spin wave. (Note that although there are also spin waves with $\lambda \approx L$ and shorter that match the imposed periodic twist, these typically correspond to much greater excitation energies and make a much smaller contribution to the free energy response.) We have labeled the helicity modulus with a free energy density label F for reasons that will shortly become apparent.

Because of the relative algebraic ease of working with inversion compared to small specific twists in the range above, FBJ introduce *antiperiodic boundary conditions* across one lattice direction as equivalent to an average twist of $|\nabla\phi| = \pm\pi/L$ between planes of spins perpendicular to the twisted dimension. This leads to

$$\Upsilon_F(T) = \lim_{L\to\infty}\left(\frac{2L^2}{\pi^2}\right)[F_a(T,L) - F_p(T,L)], \tag{3}$$

where $F_a(T,L)$ and $F_p(T,L)$ are the free energy densities of the lattice with antiperiodic or periodic boundary conditions in one chosen direction (and normal periodic boundary conditions in the rest).

There is something very interesting and perhaps unexpected about this particular choice and definition. Let us consider its implications for O(2) models and O(3) models separately. In O(2) the spins have an orientation described by a single angle (or, equivalently, an order parameter phase for, e.g., superfluids). Imposing a twist across a lattice dimension by adding or subtracting an angle to all the angles of the *boundary* spin periodic images produces a boundary condition that can be satisfied by *multiple* twisted configurations, not just the one that corresponds to a true twisted susceptibility associated with a twisted spin field of definite axis and handedness that is then permitted to smoothly vanish. The helical twist angles that smoothly connect across the lattice to satisfy the particular twisted boundary condition (such as might be imposed in an actual Monte Carlo computation) are unique only to within an arbitrary integer multiple of 2π. Also, the same relative twist angle can be reached by means of a *left-handed* or a *right-handed* twist distributed across the lattice.

For arbitrary relative twist angles, let us try to understand the relative contribution to equilibrium of the left- and right-handed twists that connect smoothly across the lattice. Let us by convention observe the lattice from a perspective such that the smallest in magnitude of the possible twist angles imposed on the boundary spins, $\Theta \leq \pi$, is right handed (positive). Let us define

$$\nabla\phi_r = \Theta/L, \tag{4}$$

$$\nabla\phi_l = (\Theta - 2\pi)/L, \tag{5}$$

to be the average *right*- and *left*-handed interlayer spin gradients across the twisted direction that corresponds to a particular (right-handed) twist angle Θ. Note that $\nabla\phi_r$ is the smaller of the two possible interlayer angles, but we will assume that $L \gg 2\pi$ is large enough that both of them are "small angles" in the sense that $|\nabla\phi|^2 \gg |\nabla\phi|^4$.

We can consider each of these separately to gain some insight into the relative likelihood of quenching into one or the other of the possible handednesses in a Monte Carlo computation. Below T_c the systems is "stiff"—it has a nonzero helicity modulus—and

$$\Delta F_r(\Theta) \approx \frac{1}{2}\Upsilon_F(T)(\nabla\phi_r)^2, \tag{6}$$

$$\Delta F_l(\Theta) \approx \frac{1}{2}\Upsilon_F(T)(\nabla\phi_r)^2, \tag{7}$$

where $\Delta F_r < \Delta F_l$ except at $\Theta=\pi$ where $\Delta F_r = \Delta F_l$. Chiral symmetry is broken—there is a gap between the right-handed (small-angle) and left-handed (large-angle) free energies that gradually vanishes as $\Theta\to\pi$. It costs more free energy to twist the system around to a given angle Θ "the long way" (or through additional multiples of 2π), which tends to suppress the mixing of unwanted helicity states that match the given boundary twist when the gap is large.

If $\Theta=\pi$, though, chiral symmetry is technically restored—there are two chiral states of distinct helicity with the same free energy. Nevertheless, we expect to observe only *one* of them in any given "experiment" (e.g., Monte Carlo quench) because the *ergodicity* of the system should be broken—in order to go from a left-handed twist of π to a right-handed twist of π the system has to go through intermediate states of much higher energy that are correspondingly improbable. It basically must accumulate a helical twist of at least 2π across a distance much less than L—effectively a "defect plane"—which must then grow across the lattice).

Switching helicity states below T_c in a system with a constrained boundary spin rotation of π is thus an *Ising*-like behavior—similar to the breaking of ergodicity that occurs when quenching an Ising model to a state of broken symmetry and ergodicity below its T_c. However, it is being observed in a *continuous* spin model.

In a continuous spin model, there is obviously no free energy barrier to a uniform rotation applied to all spins as the microscopic Hamiltonian is symmetric under rotations. In a Monte Carlo computation of such a model for a finite system, the order parameter will slowly wander around and sample different directions due to local thermal spin fluctuations or the application of the importance sampling Markov process may be [as mentioned in FBJ and studied in detail in Ref. 13 for O(3) spins]. However, in a system quenched to a state with a boundary twist of π the *handedness* of the twist it quenches to is likely to persist for much longer (divergent) timescales.

Above T_c there is enough free energy to accommodate states with *mixed* helicity and one expects to find domains with locally distinct helicity smoothly intertwined throughout the lattice for any imposed relative boundary twist angle Θ. The system is no longer "stiff."

Finally, *at* T_c (our region of interest) things are maximally complex. For a finite-size lattice, the system is weakly stiff (as the order parameter is nonzero but very small, vanishing as $L^{-\beta/\nu}$ as $L\to\infty$). We therefore expect $\Delta F_r < \Delta F_l$ up to $\Theta=\pi$ as above (where we are of course referring to these quantities evaluated for a finite-size lattice with the intent of using finite-size scaling theory later) but *now* as the gap $\Delta F_l - \Delta F_r$ narrows we can no longer presume that mixing is suppressed and the distinct quadratic forms of ΔF_l and ΔF_r are maintained. Basically, it is by no means clear that the presumed quadratic form of ΔF for small $\nabla\phi$ will be maintained for a relative twist angle of $\Theta=\pi$ where the free energy can include the entropic contribution from states of mixed helicity *even* if $\nabla\phi$ remains small.

In any event, for an O(2) spin system it is expected that the use of spin inversion in place of a twisted boundary condition with specific handedness will have little effect on the practical computation of a helicity modulus and its critical behavior. Whether the system samples left-handed, right-handed, or mixed helicity states to achieve the inversion, the inversion is exactly equivalent to a physical twist of the spins through an angle of π of either handedness, so the definition of helicity modulus *per se* as proportional to the free energy response to imposing an actual twist on the spin system is left intact by Eq. (3).

The same is *not true* for O($n>2$) spin systems. Helicity for spin dimension $n>2$ systems is *very different* in certain respects from helicity in $n=2$ systems (whatever the underlying lattice dimensionality).

Consider an O($n\geq 3$) spin system. A boundary twist through a given (by convention right-handed) twist angle $\Theta\leq\pi$ now has to be referred to a specified *axis of rotation* which *may or may not* be aligned with the nascent order parameter of a finite lattice at its critical temperature. Indeed, over time the order parameter direction itself will drift[13,14] as the lattice is sampled while in general the twist axis and angle will remain fixed. This must be compared to an $n=2$ spin system where the "twist axis" can be thought of as being fixed perpendicular to the plane in which the spins (and nascent order parameter) lie.

Still, this sort of twist is at least qualitatively similar to that of O(2); the boundary twist still has a specific handedness with respect to the twist axis and the energy of the lattice will still be lowest when the overall twist is distributed as an average rotation of $\nabla\phi_r=\Theta/L$, which corresponds to the smallest interlayer gradient that appropriately matches the imposed boundary twist angle. One still expects the free energy of a state with the larger interlayer gradients $[\nabla\phi_l=(\Theta-2\pi)/L$ and higher multiples of $2\pi]$ to be larger, with a gap that makes quenching to or sampling the larger-angle configurations less likely for $\Theta\ll\pi$, at least below T_c.

Even here, though, there are differences as well. For example, for $n\geq 3$, spins that happen to be (nearly) aligned with the twist axis *do not change* (much) as they are rotated about it, where spins that happen to be perpendicular to the twist axis can change a great deal. The distribution of the energy changes associated with bonds between layers along the twisted lattice dimension is thus very different—in particular the interlayer bond energies where one spin happens to be aligned with the rotation axis do not change at all, a result that is not possible in an O(2) lattice, where the rotation axis is "perpendicular" to the spin plane and interlayer bond energies always change by a nonzero amount.

This seems to be intuitively related to the additional freedom afforded by the extra spin dimension, which is sufficient in other contexts to prevent e.g. the formation of Kosterlitz-Thouless type[15] (long-range and short-range order) phase transitions for $n\geq 3$ spins in two spatial dimension lattices. The spins have more ways to reorient to accommodate *either* the long- or short-angle interlayer spin gradient with only small local energy differences between them. Although the additional mixing thus expected is interesting as a *qualitative* difference, this is the sort of smooth detail that one expects to see reflected in the actual details of the computations of the critical exponents and hence may not be a problem to the theory.

The most important difference, however, is a group-theoretic one and may *be* a problem to the theory. Antiperiodic inversion of a boundary layer is an *improper rotation*—it is not in SO(3), the rotation group of the sphere. It therefore cannot be related to *any* specific proper rotation or twist about *any* axis in O(3) (or any odd-n) model. Only for even spin dimension—e.g., $n=2$—is inversion in SO(n) and hence equivalent to a direct rotation of the boundary layer spins. So the definition of helicity in Eq. (3) above is *technically incorrect* for odd $n>2$ spin systems, specifically $n=3$.

This is an extremely interesting observation. Helicity is associated with small "infinitesimal" rotations $\nabla\phi$ successively and homogeneously applied to all the spins in any given transverse layer, accumulating across the lattice to a finite actual rotation of the boundary layer relative to the starting point. Inversion in odd-n dimensions changes the orientation of the coordinates and hence is not an acceptable "helical" transformation.

There is also a *topological* element to the problem posed by the use of inversion for rotation. The imposition of an antiperiodic boundary condition (or for that matter a twisted boundary condition) on a three-dimensional lattice of O(3) spins effectively causes the lattice to have a nonzero *topological charge* of either sign that we naively expect to be of order L as it should be of the order of the average spin flux fluctuation through a boundary surface with L^2 spins (consider a binomial estimate of the variance of the total perpendicular spin, for example, in a state without long-range order where the average spin in any direction is zero).

Note that this topological charge is identically *zero* by construction for spin systems with periodic boundary conditions, as the net spin flux into the volume on (say) the left-hand surface always flows out through the right-hand one. From one point of view, then, the increase in free energy associated with antiperiodic boundary conditions derives from a computation of the scaled interaction energy of a (topological) charge-charge interaction along the antiperiodic direction and might not necessarily have *any direct connection* with the energy change that results from an actual twist through an angle π with particular handedness. This is a very interesting observation, as a number of studies have directly investigated the O(3) model in particular for signs that topological charge plays an important role in the order-disorder phase transition.[7–11]

This does not alter the primary results of FBJ or the many derived Monte Carlo or algebraic results for the O(2) model, but it is a point of some concern for O($n>2$). At the very least it is clear that utilizing antiperiodic boundary conditions in definitions used to compute relations associated with actual *helicity*—involving an actual twist of definite handedness across a lattice direction—is not *a priori* justified. One of the greatest surprises of the work we present is that it appears to work *anyway*.

In preliminary computations with an actual small twist of definite handedness[16] results were obtained could not be reconciled with a purely quadratic form out to $\Theta\approx\pi$ (which is still a very small twist interlayer twist angle). Significant (numerically resolvable) deviations were observed even for angles $\Theta\lesssim\pi/2$, making it very difficult to accurately fit a quadratic form to extract a reliable estimate of the helicity modulus for finite-size scaling. This was a strong motivation for an extended and careful consideration of the problem, accompanied by very-high-precision computations (this work), and a figure is presented below (Fig. 2) illustrating the problem.

III. ENTHALPIC HELICITY MODULUS

The definitions above are of no direct use in an importance sampling Monte Carlo calculation because one cannot directly compute the free energy density F. However, the enthalpy density in zero external field is just the average internal energy per spin, E, and this quantity is trivial to evaluate at very high precision. To facilitate a Monte Carlo examination of helicity our first job is to define an equivalent "helicity modulus" for the enthalpy $\Upsilon_E(T,L)$ and determine its expected critical scaling (following the general form of the FBJ derivation).

All the arguments used by FBJ to determine the asymptotic (large L, small $t=|T-T_c|/T_c$) form of $\Upsilon_F(T,L)$ are still valid for $\Upsilon_E(T,L)$; one expects E to be an even function of the twist gradient (for twists $\Theta\leqslant\pi$ of either handedness) and one expects the critical scaling to be determined by comparing the leading-order terms in dimensionless expansions of the enthalpy difference. Thus,

$$\Delta E(\Theta)\approx\frac{1}{2}\Upsilon_E(T)(\nabla\phi)^2, \tag{8}$$

where $\Delta E(\Theta)$ is the change in internal energy per spin caused by twisting the boundary conditions through the angle $\Theta\leqslant\pi$ with either handedness. From this obvious substitutions yield

$$\Upsilon_E(T)=\frac{2L^2}{\Theta^2}\Delta E(\Theta). \tag{9}$$

The basic scaling postulate for the singular part of the enthalpy density is that it have the form

$$E\sim l^{\omega}X(x)=l^{\omega}X(l^{\theta}\dot{t}), \tag{10}$$

where $l=L/a\to\infty$ (with a the lattice constant), $X(x)$ (which may depend on the twist angle Θ) is a function of the single variable x, and where for simplicity we assume a shifted reduced temperature that scales to the true reduced temperature like $\dot{t}=t+\frac{b}{l^{\lambda}}$.

Following the finite-size scaling postulate that finite-size effects can only depend on the ratio $L/\xi(T)$,[17] we first obtain

$$\theta=1/\nu. \tag{11}$$

If we insist that in the $l\to\infty$ limit we must reproduce the correct bulk scaling

$$E\sim t^{1-\alpha}, \tag{12}$$

then equating the leading powers of t in $X(x)$ yields

$$X(x)\sim X_{\infty}x^{1-\alpha} \tag{13}$$

to leading order for any value of Θ (although there clearly must be different Θ dependence in the higher-order terms). Similarly, eliminating the l dependence yields

$$\omega=-(1-\alpha)\theta=\frac{-(1-\alpha)}{\nu}. \tag{14}$$

Subtracting the two leading-order terms to obtain the enthalpy difference, we can imagine that higher-order terms combine to yield the form

$$X_{\Theta}(x) - X_0(x) = Y_{\infty}x^{-\phi} + \cdots \quad (15)$$

and substituting

$$\Delta E(\Theta) = \frac{1}{2}\left(\frac{\Theta}{L}\right)^2 \Upsilon_E(T) \sim l^{-2}\Upsilon(t) \sim l^{\omega}Y_{\infty}x^{-\phi} \sim Y_{\infty}t^{-\phi}l^{\omega-\theta\phi}. \quad (16)$$

This requires that

$$-2 = \omega - \theta\phi, \quad (17)$$

which can be rearranged into

$$\phi = 2\nu - 1 + \alpha. \quad (18)$$

Last we relate this back to the reduced temperature t to obtain

$$\Upsilon_E(t) \sim t^{\upsilon_E} \sim t^{-\phi}, \quad (19)$$

with the critical exponent

$$\upsilon_E = -\phi = 1 - 2\nu - \alpha. \quad (20)$$

This is the critical exponent we expect to measure in the work below and can be contrasted with the free energy helicity exponent derived by FBJ (following the same procedure as above, but with a limiting form of the free energy density of $t^{2-\alpha}$ instead of $t^{1-\alpha}$):

$$\upsilon_F = 2 - 2\nu - \alpha = 1 + \upsilon_E, \quad (21)$$

where we can see that the *only* difference in the critical scaling is the extra power of t that appears in the proper helicity modulus Υ_F, which in turn comes from the different leading order t dependences in the first nonanalytic term of the underlying free energy densities. This difference suffices to make $\Upsilon_E(t)$ singular at $t=0$ where $\Upsilon_F(t)$ vanishes with a nonanalytic cusp. In the end this is a further *advantage* in a Monte Carlo calculation, as it is far easier to fit a leading-order singularity than a small-exponent cusp with the inevitable confluent corrections, a problem that has plagued the accurate computation of the critical exponent α from a direct finite-size scaling fit of the (cusped) specific heat.

In the sections below we will review the numerical methodology of our direct measurement of υ_E using finite-size scaling theory.[17] Following this we will present a discussion of the results obtained from its application.

IV. COMPUTATION

Ignoring for the moment the fact that antiperiodic boundary conditions are not equivalent to a helical twist of π, we directly computed the helicity modulus from the FBJ expression (modified for the use of enthalpy rather than free energy)

$$\Upsilon_E(T_c,L) = \left(\frac{2L^2}{\pi^2}\right)[E_a(T_c,L) - E_p(T_c,L)] \quad (22)$$

at the critical temperature. We *also* computed the helicity modulus *directly from its fundamental definition* by computing $E(\Theta \leq \pi)$ for various angles in the range $[0,\pi]$ and fitting the results as best as possible to

$$\Delta E(\Theta) \approx \frac{1}{2}\Upsilon_E(T)(\nabla\phi)^2. \quad (23)$$

Both computations utilized a unique Monte Carlo handling of the boundary conditions. To speed convergence and maximize sampling efficiency, the Monte Carlo computation of Eq. (22) was performed with a modification of the Wolff cluster method[18] for O(n) spin models that works for either normal or inverted (antiperiodic) boundary conditions. A flip plane is selected, a random spin is flipped, and an Ising-like accept-reject decision is made along all connected bond directions (one time only per bond) to determine whether or not to flip the spin and include it in the flipped cluster. The process is repeated for any flipped spins until all the cluster stops growing (all boundary bonds have been tested). By applying an inversion within the computation of energy differences when considering a flip for a bond that crosses the antiperiodic boundary, it was possible to directly and accurately generate and sample equilibrium antiperiodic spin configurations (effectively permitting flipped clusters to correctly grow across the antiperiodic boundary).

To compute Eq. (23) we used a modified heat-bath Monte Carlo method where we instead applied a uniform rotational twist of fixed angle $\Theta \in [0,\pi]$ to nearest-neighbor spins that lie across the twisted boundary. At each boundary all spins thus saw a uniform local environment, but one that *smoothly* realized an actual Möbius twist across the twisted toroidal direction. Both computations were carried out at the critical temperature.

The critical temperature $T_c = 1.44\,298 \pm 0.000\,02$ used was directly determined in this computation to be associated with an apparent fixed point in the fourth-order complaint flow (Binder parameter)[19] at least up to $L=96$, the maximum lattice size used in this computation. This leads to a critical coupling of $K_c = 0.693\,01$, in excellent agreement with earlier results.[12,13,20–25] All Monte Carlo results are supported by reliable error estimates determined using the methodology described in Ref. 13.

We accumulated antiperiodic (a) and periodic (p) sample data from which we obtained $E_{a,p}(T_c,L)$ to a relative accuracy of 10^{-5} or better for L ranging from 8 to 96 (more than a log decade). From these data we were able to compute $\Upsilon_E(T_c,L)$ to very high precision using Eq. (22).

We simultaneously accumulated and evaluated $M_{a,p}(T_c,L)$ (the order parameter) to a relative accuracy of 10^{-4} or better. By also accumulating and evaluating the average moments of E_p and M_p we were able to compute most of the thermodynamic quantities of interest and use finite-size scaling to try to evaluate their associated static critical exponent ratios: e.g., α/ν or β/ν.

We were somewhat more lax in the precision demanded of the heat-bath computation of the energy δ's resulting from an actual twist angle Θ in the periodic boundary condition across a toroidal direction for use in Eq. (23). This is because (as is clear from the results portrayed below) this form *cannot be fit* to a quadratic form except at very small $\Theta \lesssim \pi/2$. This leaves one with the uncomfortable problem that, *even* for small Θ, as one obtains ever higher precision by sam

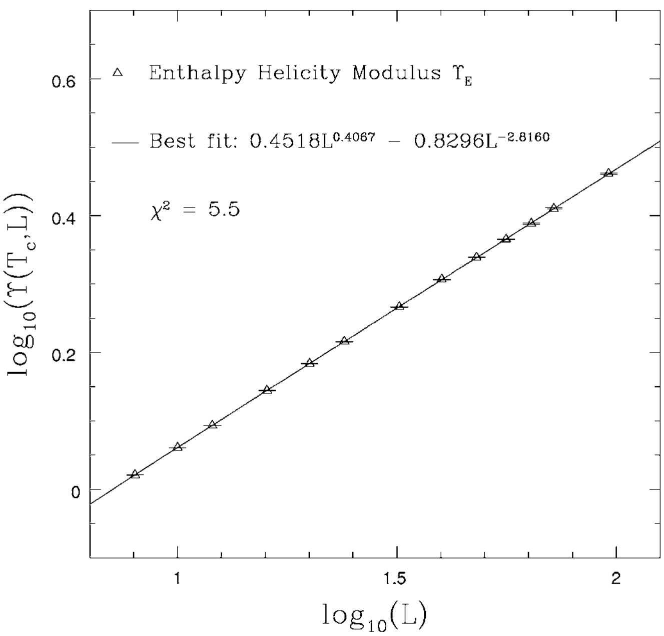

FIG. 1. $\log_{10}$-$\log_{10}$ plot of $\Upsilon(t=0,L)$ and its best fit evaluated using Eqs. (22) and (24) for lattices with $L=8,10,12,16,20,24,32,48,56,64,72,96$.

pling for longer and longer times, the χ^2 of a quadratic fit gets *worse*.

While one can at least try to add correction terms to the fit with *reasonable* forms to see if one can still extract estimates for the (singular) critical exponent ratios, in the absence of any theoretical guidance this makes the accuracy of any result at all obtained from these curves by means of such a process questionable. Nevertheless, the curves themselves are *very interesting* in what they teach us *qualitatively* about the relationship between the actual helicity modulus (evaluated from real twists of definite handedness) and the "inversion" modulus determined using an antiperiodic boundary twist.

V. RESULTS

For reasons mentioned above and analyzed in greater detail below, the critical exponent v_E was extracted by fitting $\Upsilon(T_c,L)$ as evaluated from Eq. (22) [as opposed to Eq. (23)] for various lattice sizes to the finite-size scaling form

$$\Upsilon_E(T_c,L) \approx Y_0 L^{v_E/\nu} + Y_1 L^{-x} + \cdots, \tag{24}$$

with nonlinear regression. Here we do have some theoretical guidance as to a reasonable form for confluent corrections. The second term is a confluent correction influenced primarily by the high-precision low-L data in order to reliably fit the asymptotic singular form; it smoothly vanishes at larger L. The data and best fit are shown in Fig. 1. The best regression fit is

$$\Upsilon_E(T_c,L) \approx 0.4518L^{0.4067} - 0.8296L^{-2.8160} + \cdots, \tag{25}$$

with $\chi^2=5.5$. The relative precision of the points that are being fit, obtained using an analysis of results from many independent runs, is less than 0.3%.

We fit $E(T_c,L)$ [which is the usual energy per spin computed from a lattice with normal periodic boundary conditions $E_p(T_c,L)$] directly:

$$E(T_c,L) = E_\infty + E_0 L^{(1-\alpha)/\nu} + \cdots$$
$$\approx -0.9896 \pm 1.7225L^{-1.5974} + \cdots \tag{26}$$

(with $\chi^2=18.5$). The relative precision of the data fit is 0.001% or better. This is a remarkably good fit given the extraordinary accuracy of the data and the fact that there are no confluent correction terms used. The good fit without confluent corrections is a reasonable indication that our estimate for the critical temperature is at least not a *bad* one.

We fit the zero-field specific heat (evaluated from the values of $\langle E\rangle,\langle E^2\rangle,\ldots$ accumulated during the periodic boundary condition computations) to a cusp form

$$C(T_c,L) = C_\infty + C_0 L^{-\alpha/\nu} + C_1 L^{-y} \cdots$$
$$\approx 4.9511 \pm 4.1559L^{-0.1991} \pm 0.7242L^{-1.3956} + \cdots \tag{27}$$

(with $\chi^2=1.8$), where the fit requires a confluent correction and where relatively large energy susceptibility error estimates (0.2%) were determined by a jackknife procedure.[26] The larger error estimates are likely responsible for the relatively small χ^2. It is worth noting that this is a *very difficult result* to fit *reliably* in the sense that the answer obtained is independent of the assumed cusp form and the number and type of confluent correction terms.

Although the helicity modulus is computed in part from $E_p(T_c,L)$, it *also* involves the computation of $E_a(T_c,L)$ (an independent quantity) and hence these two results are independent (in the specific sense that one is not linearly dependent on the other). Similarly, $E_p^2(T_c,L)$ (the enthalpy density squared averaged over many Monte Carlo configurations) and the derived specific heat is a quantity that is independent of $E_p(T_c,L)$ and $\Upsilon(T_c,L)$. In each of these quantities there is unique information that measures the average energy per spin, the additional energy per spin caused by a twist, and the average size of fluctuations in the energy per spin, respectively. The results of these three *distinct* results from the computations can then be compared.

We also performed a *direct* computation of $E(\Theta,T_c,L)$ [to fit according to Eq. (23)] for a range of Θ. Typical results are presented in Fig. 2 for $L=16$ and 32. It is easy to see from these figures that although the energy response is roughly quadratic for *small* total twist angles $\Theta \ll \pi$, it deviates significantly from quadratic behavior well before $\Theta=\pi/2$.

It is important to note that $\nabla\phi=\Theta/L$ is a *small angle* throughout the entire displayed range for *both* curves and that (for a given value of Θ) it is *half* the size for $L=32$ that it is for $L=16$. Yet the curves appear to deviate from quadratic form in about the same way at about the same angle Θ independent of L. It seems that Θ is the angle that must be "small" for Eq. (23) to hold, *not* $\nabla\phi$, when both of them are small enough that the spin-spin interaction energy is expected to have a dominant term quadratic in the angle in between.

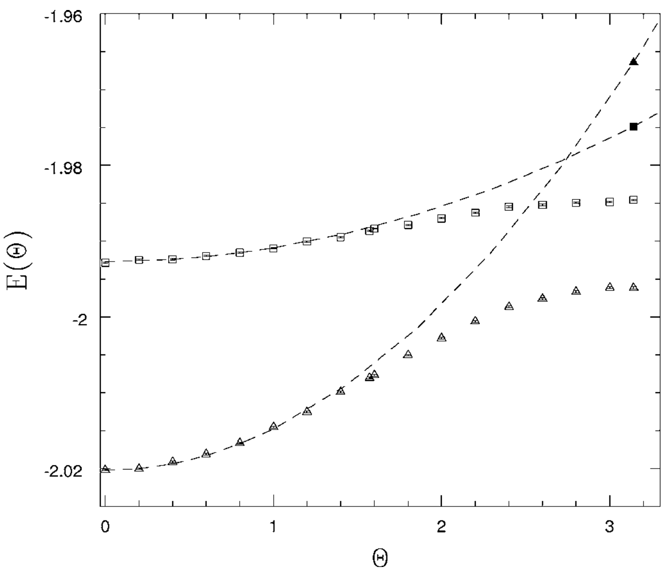

FIG. 2. Direct computation of $E(\Theta,T_c,L)$ for $L=16$ (triangles) and $L=32$ (squares) at $T_c=1.44298$. Quadratic fits of Eq. (23) to the small-angle portions are given as dashed curves. The two associated $E_a(T_c,L)$ are given as a solid triangle and square on the same graph. Note well that they lie *precisely* on the extrapolated quadratic curves.

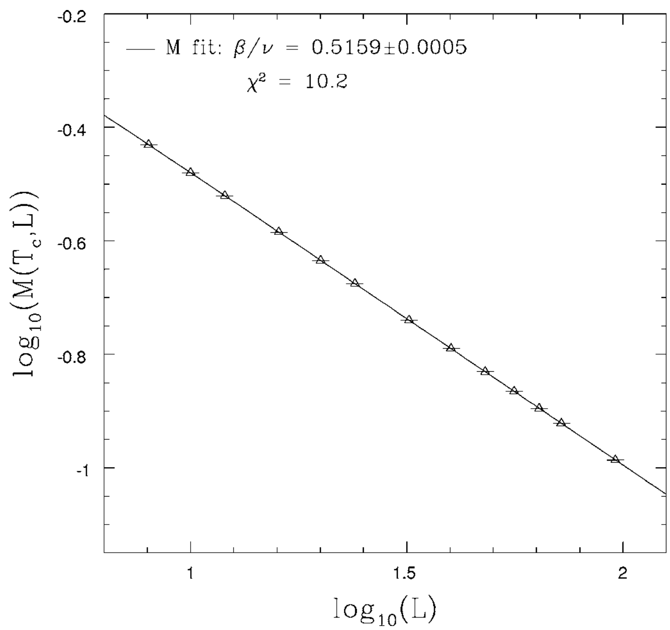

FIG. 3. $M(T_c,L)$, and its best fit, presented on a $\log_{10}$-$\log_{10}$ scale. We fit the ten points $L=16,20,24,32,48,56,64,72,96$ to an empirical form that includes an exponential confluent term to extract the asymptotic exponent ratio $\beta/\nu\approx0.5159\pm0.0005$, although the unfit points $L=8,10,12$ are also included in the figure.

The quantity that is directly controlled by Θ independent of L is the free energy gap between F_r and F_l as described above. When this gap is large, one expects to see no helical mixing—the system will nearly always select configurations that increment the average spin angle between planes in the direction of the smaller in magnitude of Θ and $\Theta-2\pi$. As $\Theta\to\pi$, this gap goes to zero (at T_c) in the sense that intermediate states of small free energy cost connect the two helicities. We therefore interpret the nonquadratic behavior as evidence that the mixing of states of opposite handedness occurs as described above, causing the free energy to be reduced because of the higher entropy of the accessible states or (if you prefer) because the additional degrees of freedom afforded in the O(3) Goldstone modes allow the system to find better ways of accommodating the imposed twist than just cumulating interlayer helicity in a uniform way.

This figure *also* shows one of the greatest surprises of the entire computation. We plot the energy $E_a(T_c,L)$ [obtained to use in Eq. (22)] above the twisted $\Theta=\pi$ point on each curve (solid triangle and square). Note that this energy results from forcing *antiperiodic* (not twisted) boundary conditions.

The result is *extremely interesting*. The energies corresponding to antiperiodic boundary conditions appear to lie *exactly* on the extrapolated quadratic fits to the energies associated with the small Θ twists. As noted above, using an antiperiodic boundary condition to evaluate the helicity modulus is mathematically a *mistake* in O($n>2$) where inversion of the spin coordinates of all the boundary spins is not equivalent to *any* rotation uniformly applied to all the spins. It is not, in fact, a "helicity modulus" at all in O(3). In any event, its apparently location precisely on the extrapolated quadratic helicity response curves is something that as far as we know is not yet theoretically explained or predicted.

Finally, we fit the order parameter data *only* for the range $L=16-96$ to the empirical form

$$M(T_c,L)=M_0L^{-\beta/\nu}+M_1e^{-L/L_0}+\cdots$$
$$\approx1.0879L^{-0.5159}\pm0.0225e^{-L/2.7566}+\cdots \quad (28)$$

(with $\chi^2=10.2$). The fit data had a relative precision of better than 0.01% (absolute errors around 1×10^{-5} throughout). The data and the best fit are displayed in Fig. 3. Note well that on this scale the errors are all *much* thinner than the width of a line.

Any attempt to fit *all* the data from $L=8$ to 96 with an algebraic form with or without an exponential correction term either failed outright (yielding a very large χ^2) or required that we fit only data for, e.g., $L>32$ to get a χ^2 that was only *slightly* large and which predicted more or less the same value for β/ν. There are clearly significant confluent corrections required to be able to fit the data at all at this level of precision.

This is directly evident from the length scale apparent in the successful form above, which effectively compresses a whole power series of correction terms into the exponential. It directly demonstrates that there are corrections that are significant compared to the precision of the data out to at least $L=32$. The variation observed in all the different ways we attempted to fit the data are reflected in the error we assign to the best-fit estimate of β/ν (effectively reflecting our uncertainty in the best way to accommodate the corrections) as the error in the fit itself is much smaller.

VI. ANALYSIS OF THE RESULTS

Dividing both sides of Eq. (20) by $-\nu$, we obtain from our measurement the relation

TABLE I. Independent pairs of hyperscaling-based estimates of α and ν for O(3) spins on a three-dimensional lattice.

Quantity	α	ν	υ_F
$\Upsilon(T_c,L)$	−0.1327	0.7109	0.7109
$E(T_c,L)$	−0.1389	0.7130	(NA)
$C(T_c,L)$	−0.1422	0.7141	(NA)

$$-\upsilon_E/\nu = 0.4067 = 2 - \frac{1-\alpha}{\nu}. \tag{29}$$

We now have three distinct numerical relations involving α and ν: one from the helicity modulus, one from the direct scaling of the enthalpy density (internal energy per spin), and one from the specific heat. Furthermore, the helicity-based result is computed in a way that is *independent* of the direct energy-based results (which are at least partly dependent on one another, as the specific heat involves $\langle E\rangle^2$ as well as $\langle E^2\rangle$).

We can therefore assume hyperscaling to be valid for *each* result and compare the resulting values of α and ν. If they are consistent, we can conclude that hyperscaling is very likely satisfied for this model. For example,

$$\nu = \frac{1}{1-\frac{\upsilon_E}{\nu}} = \frac{1}{1.4067} = 0.7109 = (d-2)\nu = \upsilon_F. \tag{30}$$

[Note that this equation makes an explicit connection to FBJ's observation that the helicity exponent υ_F (and the associated "helicity length") may well *be* the correlation length exponent (and correlation length) for this sort of model.]

The results of this comparison are shown in Table I. The exponents are in excellent agreement; from the variation observed in this table and the observation that the result derived from the direct fit of the energy data is likely to be the most precise, one can assign a value of $\nu \approx 0.713 \pm 0.003$ and $\alpha \approx -0.139 \pm 0.009$ and conservatively conclude that hyperscaling appears to be *numerically* satisfied by this model to within about 1%. It is also worth observing that these values for the exponents are close to but not in precise agreement with the prediction of renormalization theory[27] of $\nu \approx 0.705 \pm 0.003$ for this model.

The last result of this computation to discuss is the critical scaling of the order parameter. As noted, only an exponential confluent correction (which effectively compresses a whole power series of confluent terms) succeeded in reducing χ^2 to an acceptable value for the greater part of the $\log_{10}$ decade being fit. This is not, actually, a complete surprise; it was suggested to us some time ago that finite-size scaling fits may need to be carried out over two decades of L values to accurately accommodate confluent corrections in this model.[28]

Note well that the M data (like the E data) were *extremely precise*—precise enough that one simply could not manage a "sloppy" fit to an exponential-only form without going out to $L=32$ to *begin* the fit, and even there the omission of the residual deviation resulting from the confluent exponential bumps χ^2 over the value it has for the whole range as given.

Based on this fit and observed variations from other attempted fit forms and ranges, we assign the value $\beta/\nu = 0.5158 \pm 0.0005$ to this quantity. This is in excellent agreement with the renormalization estimate[27] of $\beta/\nu \approx 0.517 \pm 0.005$. From the knowledge thus obtained of ν and β/ν we find $\beta = 0.368 \pm 0.001$.

VII. CONCLUSIONS

The primary results of this work are the direct computation of the helicity exponent υ_E, its application in the validation of hyperscaling leading to the conclusion $\upsilon_F = \nu$, and the computation of the nonhyperscaling exponent ratio β/ν. From these measurements and from scaling and hyperscaling relations we can find the rest of the critical exponents for the model.

These results are in reasonable agreement with the predictions of renormalization, although we find ν and α to be slightly higher in magnitude than previous studies using Monte Carlo or renormalization approaches. However, given the consistency of our measurements using very different methodologies and the very high precision of our data for two of them we cannot easily force our fits into agreement within their respective error estimates.

The computations presented herein also pose some new puzzles and challenges for the future. In particular is the surprising and unexpected behavior of the "antiperiodicity modulus," which one might well expect to be *different* from the actual helicity modulus in an O(3) model where inversion is an *improper* transformation across the lattice toroid, one that cannot be accomplished by any continuous helical twist of the spin field across the lattice. We find that the finite-size scaling of the antiperiodicity modulus appears to *precisely correspond* to the extrapolation of the small-Θ results for the *actual* helicity modulus. The helicity modulus (computed by twisting the periodic boundary conditions through an actual angle with a given helicity) exhibits an expected *mixing* and *spin alignment* behavior that reduces the enthalpy cost of a twist at $\Theta \approx \pi$ from the expected and extrapolated small-$\nabla\phi$ quadratic energy dependence by close to a factor of 2, even though $\nabla\phi$ is still extremely small between any pair of neighboring spins along the twisted dimension especially for the larger lattice sizes.

This result is startling and appears as if it might have significant implications in theories where a breaking of chiral symmetry in a continuous isotropic model with spin dimension $n > 2$ is physically important. It is also fortuitous, as it permits us to evaluate υ_E to very high precision without having to worry about fitting a function that is at best only asymptotically quadratic in such a way that increasing the precision of the data inevitably makes a quadratic fit *worse* in terms of χ^2.

The antiperiodicity modulus appears to be an interesting quantity in its own right. Just as periodic boundary conditions constrain the total topological charge of the spin block studied to be *zero*, imposing an antiperiodic inversion of the boundary conditions across one lattice dimension constrains the total topological charge of the spin block to be *nonzero*. The effective period of the lattice in the twisted and inverted dimension becomes $2L$, in alternating layers of opposite topological charge sign, so that the energy increase can be interpreted as due to the *interaction of topological charge* in the model between blocks centers separated by a scale length L—basically *capacitance*.

Holm and Janke[9] have published a convincing study that shows that the O(3) transition is not associated with any sort of divergence in hedgehog defect (topological charge) density, and both Kamal and Murthy[10] and more recently Motrunich and Vishwanath[11] have showed that an order-disorder transition [with different critical exponents than the O(3) model] is possible in constrained O(3) models with hedgehogs suppressed. Nevertheless, the remarkable position of the antiperiodic and topological charge energy on the extrapolated helicity energy curves suggests that there is a close connection between the scaling of helicity and hedgehog topological charge-pair energies and the convincing demonstration that $v_{\mathrm{F}} \approx \nu$ for this model in turn connects helicity and *hence* topological charge with the scaling length of the system and hence the advent of order. This is a puzzle worthy of further examination.

This work has therefore opened up a whole range of questions that will need to be addressed by future research. They include the following.

(i) The effect of imposing antiperiodic (or twisted) boundary conditions across two and three lattice dimensions, not just one. Doing so might be expected to *significantly change* the properties of the observed block-scale topological charges. In particular, if antiperiodic conditions are imposed on all three lattice dimensions, the *ferromagnetic* lattice-scale block can support true hedgehog configurations, with outgoing spin flux on all eight faces, interacting with neighboring blocks of the opposite topological charge. Loops of spin flux also become possible.

(ii) Quantitative studies of topological charge (utilizing the usual methods for determining the topological charge of unit cubes of spins) at various lattice length scales in the presence of a twisted or antiperiodic boundary conditions.

(iii) Extending the methods introduced in this study to continuous models with different lattice dimension d and spin dimension n. In higher dimensions both the notion of a topological charge and the use of, e.g., spinors instead of spins (in association with rotations versus antiperiodic boundary conditions) become potentially more interesting, especially to field theorists.

(iv) Dynamical models. For example, computations involving the preparation of a lattice with a twist of π with a particular handedness across the lattice via a superimposed, continuously varying spin field and its relaxation to a mixed helicity state when the twisted field is suddenly set to zero or preparing a lattice with a given initial distribution of topological charges and observing its relaxation.

As noted in the Introduction, this general problem is of interest in many areas of physics, not just condensed matter. The methodology used in this work represents an interesting approach to studying the connection between helicity, topological charge, and the order-disorder phase transition in continuous spin models.

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