A New Universality at a First-Order Phase Transition: The Spin-flop Transition in an Anisotropic Heisenberg Antiferromagnet

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Abstract. A great triumph of statistical physics in the latter part of the 20th century was the understanding of critical behavior and universality at second-order phase transitions. In contrast, first-order transitions were believed to have no common features. However, we argue that the classic, first-order “spin-flop” transition (between the antiferromagnetic and the rotationally degenerate, canted state) in an anisotropic antiferromagnet in a magnetic field exhibits a new kind of universality. We present a finite-size scaling theory for a first-order phase transition where a continuous symmetry is broken using an approximation of Gaussian probability distributions with a phenomenological degeneracy factor “$q$” included, where “$q$” characterizes the relative degeneracy of the ordered phases. Predictions are compared with high resolution Monte Carlo simulations of the three-dimensional, $XXZ$ Heisenberg antiferromagnet in a field to study the finite-size behavior for $L \times L \times L$ simple cubic lattices. The field dependence of all moments of the order parameters exhibit universal intersections at the spin-flop transition. Our Monte Carlo data agree with theoretical predictions for asymptotic large $L$ behavior. Our theory yields $q = \pi$, and we present numerical evidence that is compatible with this prediction.

The agreement between the theory and simulation implies a heretofore unknown universality.

1. Introduction

Finite-size scaling for transitions between phases with discrete numbers of states is now relatively well established for both first-order and second-order phase transitions. This powerful framework has been extremely successful at describing phase transition behavior in the thermodynamic limit from Monte Carlo data for finite-size systems \cite{1, 2, 3, 4, 5, 6, 7}. The first-order, field driven transition in the 2-dimensional Ising model below its critical point, arguably the simplest case of a first-order transition, was studied using Monte Carlo simulations by Binder and Landau \cite{4} who found that the probability distribution of the order parameter at the transition in a finite system could be rather well described by the sum of Gaussians representing the two coexisting states. For the temperature driven first-order transition in the $q$-state Potts model a similar theory could be used, but a factor of “$q$” must be included in the Gaussian representing the $q$-fold degenerate ordered state \cite{5}. Monte Carlo simulations of the $q = 10$ Potts model on $L \times L$ lattices verified this finite-size behavior \cite{6}.
Figure 1. Spin configurations for different phases in the XXZ Heisenberg model in an external field. Spin configurations of the two sublattices are shown for the (a) antiferromagnetic (AF); and (b) spin-flop (SF) phases. $\theta_{SF}$ is the angle that the spins make with respect to the applied field.

For a first-order phase transition where a continuous symmetry is broken, there were neither theoretical predictions nor good data from simulations describing the finite-size behavior. Here, a “fruit fly” model is thus necessary to help provide guidance, and the uniaxially anisotropic, three-dimensional (3D) Heisenberg antiferromagnet in an external field, $H$, is exactly such a candidate model. Substantial interest has been shown in this model for decades, largely about the general features of the phase diagram and ordered structures and the nature of the multicritical point identification [8, 9, 10, 11, 12, 13, 14, 15, 16, 17].

2. Model and methods

2.1. Three-dimensional anisotropic Heisenberg model

The uniaxially anisotropic Heisenberg antiferromagnetic model in an external field has elicited great interest for many years [11, 14, 15, 16, 17, 18]. The Hamiltonian of this model is given by,

$$\mathcal{H} = J \sum_{\langle i,j \rangle} [\Delta(S_i S_j^x S_j^x + S_i S_j^y S_j^y) + S_i^z S_j^z] - H \sum_i S_i^z,$$

where the classical spins $S_i$ are unit vectors with components $(S_i^x, S_i^y, S_i^z)$ on sites $i$ of a simple cubic lattice of linear size $L$, and $J > 0$ is the exchange coupling between nearest-neighbor pairs of spins. $\Delta$ is the uniaxial exchange anisotropy, which we set to $\Delta = 0.8$. An external magnetic field $H$ is applied along the $z$-axis which is the easy axis of the model. The first summation is over all $\langle i,j \rangle$ pairs of nearest-neighbor sites and the second summation is over all $N = L^3$ spins on the lattice. (Recent high-resolution simulations of this model with $\Delta = 0.8$ near the bicritical point provide a good starting point for the current study.)

The phase diagram has been studied by various methods for many years, e.g. renormalization group [19] and mean field theory [20]. We now believe that an antiferromagnetic (AF) phase exists at low temperature and low field, where the nearest-neighboring spins point in opposite directions along the axis given by the anisotropy (as shown in Fig. 1(a)); a spin-flop (SF) phase exists at low $T$ and higher $H$, in which the spins are tilted with continuous rotational symmetry about the field direction (see Fig. 1(b)). (The angle $\theta_{SF}$ depends upon the strength of the magnetic field.) In addition, a paramagnetic (P) phase with no long range order exists at high $T$ and/or at high $H$.

Both the SF-to-P and the AF-to-P phase transitions are of second-order. They belong to the XY and the Ising universality classes, respectively; but the phase transition between the AF and SF phases is first-order. The point $T = T_b$ where the three phases meet was determined to be a bicritical point in the three-dimensional (3D) Heisenberg universality class. Fig. 2 shows the corresponding phase diagram in the neighboring area of the bicritical point for $\Delta = 0.8$. In earlier work, the spin-flop boundary for the anisotropic Heisenberg antiferromagnet in an applied field was located rather precisely [16, 17], consequently this model is actually a fertile
Figure 2. Phase diagram for the 3D anisotropic Heisenberg model in an applied magnetic field, $H$, near the bicritical point [17]. Both the temperature, $T$, ($k_B$ is Boltzmann’s constant) and the external field are normalized by the exchange constant $J$. The order parameter for the antiferromagnetic phase is $\tilde{m}_z$ and for the spin-flop phase is $\vec{\psi}$. The $z$-component of the uniform magnetization is $m_z$.

testing ground for the study of finite-size effects at a first-order transition where a continuous symmetry is broken.

The phase diagram near the bicritical point in the temperature $T$ and field $H$ plane is shown in Fig. 2, where the meeting point of the three phase transition lines is estimated to be at $k_B T_b/J = 1.025 \pm 0.0025$ and $H_b/J = 3.89 \pm 0.01$ [16, 17]. Note that here we are not interested in the phase boundaries near the bicritical point but shall focus on the finite-size effects associated with the first-order transition from the AF phase to the SF phase at $T = 0.95 J/k_B$, $T = 0.80 J/k_B$, and $T = 0.60 J/k_B$ at the transition field $H^t$ which will be temperature dependent.

2.2. Monte Carlo sampling methods
For $T = 0.95 J/k_B$ two different Monte Carlo methods were used to carry out the simulations, where simple cubic lattices with even values of $L$ and periodic boundary conditions were considered. Simulations for $L \leq 60$ were first performed using a standard Metropolis algorithm [21] with the R1279 shift register random number generator [7]. Runs of length $3 \times 10^7$ MCS were performed for all lattice sizes and the number of independent runs ranged from 10 for $L = 30$ to 1035 for $L = 60$. For $L = 60$ Metropolis sampling had great difficulty tunneling between the two states on opposite sides of the spin-flop transitions. Therefore, to ensure that the sampling was truly ergodic for $L = 60$, $L = 80$ and $L = 100$, we implemented multicanonical sampling [22]. Multicanonical simulations were then performed for the entire range of sizes so that results could be compared with those from Metropolis sampling. The multicanonical sampling probability was determined iteratively for each $L$ until the multicanonical probability density $P_{\mu ca}(E)$ of the energy is “flat” enough, see Fig. 3. Then runs of length $10^7$ MCS were carried out. To determine averages and error bars a total of 100 independent runs were made for $L = 30$, and the number increased with increasing size until 900 independent runs
Figure 3. Multicanonical probability density $P_{\text{muca}}(E)$ of the energy with different iterations for $L = 100$ at $T = 0.95 J/k_B$.

were used for $L = 100$. For smaller lattices, there was agreement between the data generated using the two different sampling methods and the results could be combined for the analysis. For the multicanonical runs the Mersenne Twister random number generator was used [7]. For $T = 0.80 J/k_B$ and $T = 0.60 J/k_B$, similar multicanonical simulations as mentioned above were applied to generate data for $L = 10$ up to $L = 50$ and $L = 10$ up to $L = 40$ respectively. (Simulations were performed for smaller $L$ values for these temperatures since we found that the asymptotic size regime was reached for smaller sizes as the temperature was lowered.) Histogram reweighting techniques [23] were applied to extract thermodynamic quantities for fields near the values used in the simulations. For the largest lattices, comparisons were made between runs made at adjacent field values and reweighted results to ensure that we were not reweighting beyond the reliable range of fields.

3. Theory and quantities to be analyzed
In this section we provide a general outline of the underlying theory used to address the finite size scaling behavior near the AF to SF transition, but a more complete treatment can be found in [18].

3.1. General relations and order parameters
For small magnetic fields, i.e. $H < H^c(T)$, and low temperatures, $T$, the anisotropic Heisenberg antiferromagnet exhibits Neél-type two-sublattice order on the simple cubic (or other bipartite three-dimensional) lattices. This order is described by the staggered magnetization (with the two interpenetrating sublattices of the $L \times L \times L$ lattice denoted by indices 1 and 2 )

$$\tilde{m}_z = \frac{1}{L^3} \left( \sum_{i \in 1} S_{iz} - \sum_{i \in 2} S_{iz} \right). \quad (2)$$

For $H > 0$ there is a non-zero uniform magnetization $m_z$ (per spin)

$$m_z = \frac{1}{L^3} \left( \sum_{i \in 1} S_{iz} + \sum_{i \in 2} S_{iz} \right). \quad (3)$$

4
At the transition field, $H = H^t(T)$, a first-order phase transition occurs to the "spin-flop" phase described by a two-component order parameter involving the transverse spin components

$$
\psi_\alpha = \frac{1}{L^3} \left( \sum_{i \in 1} S_{i\alpha} - \sum_{i \in 2} S_{i\alpha} \right), \quad \alpha = (x, y).
$$

(The transition field in the thermodynamic limit is denoted $H^t$.) Both $\psi_x$, $\psi_y$ are equivalent and form the components of a vector order parameter $\vec{\psi}$ with $XY$ symmetry.

While the AF phase is two-fold degenerate ($n = 1$, one-component order parameter), in the SF phase a continuous ($XY$-model like) symmetry is broken ($n = 2$, two-component order parameter). How this difference enters in the weights is not obvious, unlike in the simpler case of the thermally driven $q$-state Potts model [24] with Hamiltonian

$$
H = -J \sum_{\langle i,j \rangle} \delta_{\sigma_i \sigma_j},
$$

where $\sigma_i = 1, 2, ..., q$ and nearest neighbors interact only if they are in the same state. In the $q$-state Potts model, the high-temperature phase is non-degenerate and the low-temperature phase is simply $q$-fold degenerate. An extra factor $q$ then appears in the weight of the low-temperature phase multiplying the Boltzmann factor. But what should this factor $q$ be when dealing with a continuous symmetry? We will simply introduce an "effective" factor $q$ phenomenologically to account for the difference in degeneracy between the phases at coexistence in the thermodynamic limit ($H = H^t$). As in the case of the Potts model, this factor leads to shifts of characteristic finite-size induced features (e.g. position of the maximum of the magnetic susceptibility or specific heat, minimum of the various cumulants, etc.). Our Monte Carlo data will provide numerical estimates for these quantities which can, in turn, be used to estimate this degeneracy factor $q$ for the spin-flop transition.

We now assume that the "equal weight rule" [5] holds for the statistical weights of the two phases, i.e. $a_{AF} = N \exp(-\Delta F_{AF} L^3/k_B T)$ and $a_{SF} = N q \exp(-\Delta F_{SF} L^3/k_B T)$, with a normalization factor $N$. Requiring $a_{AF} + a_{SF} = 1$ yields

$$
a_{AF} = \exp(\Delta F L^3/k_B T)/[q + \exp(\Delta F L^3/k_B T)],
$$

$$
a_{SF} = q/[q + \exp(\Delta F L^3/k_B T)],
$$
as expected.

### 3.2. Order parameter distribution at the transition in the thermodynamic limit

The transition between the disordered and ordered states for the $q$-state Potts model can provide some insight about the effective degeneracy factor for the AF to SF transition in the anisotropic Heisenberg model. For the $q$-state Potts model in the thermodynamic limit at the transition temperature, the probability distribution of the order parameter $P(\vec{\psi})$ is simply the sum of $q + 1$ weighted delta functions,

$$
P(\vec{\psi}) = \delta(\vec{\psi}) + \sum_{k=1}^{q} \delta(\vec{\psi} - \vec{\psi}_k),
$$

where the $\vec{\psi}_k$ are the discrete values of the order parameter in the ordered phase [25]. The first term on the right hand side of Eq. (8) represents the disordered phase and the second term represents the (degenerate) ordered phase. For the AF to SF transition a similar expression
holds except that the \( \vec{\psi} \) are continuous. An analogous expression for the spin-flop case would then be

\[
P(\vec{m}_z, \psi) = [\delta(\vec{m}_z - \vec{m}_{z,\infty}) + \delta(\vec{m}_z + \vec{m}_{z,\infty})] \delta(\psi) + \int_0^{2\pi} \delta(\vec{m}_z) \delta(\psi - \psi_\infty) d\phi, \tag{9}
\]

where the order parameter \( \vec{\psi} \) is expressed in terms of the magnitude \( \psi \) and angle \( \phi \) in the \((\psi_x, \psi_y)\) plane, and we have integrated over \( \phi \). The index "\( \infty \)" indicates that the thermodynamic limit was taken first and then the limit \( H \to H^t \). The integral simply gives \( 2\pi \), and integration over \( \vec{m}_z \) yields

\[
P(\psi) = 2\delta(\psi) + 2\pi \delta(\psi - \psi_\infty). \tag{10}
\]

This means that the relative weight of the two phases is simply \( q = \pi \! \! \! \! \! \! /2 \!

Eq. (9) merely indicates that in the thermodynamic limit and for \( H = H^t \), we have phase coexistence between pure AF phases \((\vec{m}_z = \pm \vec{m}_{z,\infty}, \vec{\psi} = 0)\) and pure SF phases \((\vec{\psi} = (\psi_\infty, \phi), \text{in polar coordinates in the } (\psi_x, \psi_y)-\text{plane}, \text{and } \vec{m}_z = 0)\). The distribution of the order parameters is simply characterized by the appropriate Dirac delta-functions. Making contact with formulation of Eqs. (6), (7), where the relative weights of the two phases at \( H^t \) was denoted by the phenomenological parameter \( q \), we find that the joint (unnormalized) distribution of the order parameters \( \vec{m}_z, \psi = |\vec{\psi}| \) becomes

\[
P_\infty(\vec{m}_z, \psi) = [\delta(\vec{m}_z - \vec{m}_{z,\infty}) + \delta(\vec{m}_z + \vec{m}_{z,\infty})] \delta(\psi) + 2q \delta(\vec{m}_z) \delta(\psi - \psi_\infty). \tag{11}
\]

The normalization constant for this distribution is

\[
N_\infty = \int_{-1}^{+1} d\vec{m}_z \int_0^1 d\psi P_\infty(\vec{m}_z, \psi) = 2 + 2q. \tag{12}
\]

From Eqs. (11), (12) we obtain the moments of both order parameters (the notation \( \langle \cdots \rangle_\infty \) means that an average over both phases at the transition point in the thermodynamic limit is taken)

\[
\langle |\vec{\psi}| \rangle_\infty = \psi_\infty q/(1 + q), \tag{13}
\]

\[
\langle \psi^2 \rangle_\infty = \psi_\infty^2 q/(1 + q), \tag{14}
\]

\[
\langle \psi^4 \rangle_\infty = \psi_\infty^4 q/(1 + q), \tag{15}
\]

\[
\langle |\vec{m}_z| \rangle_\infty = \vec{m}_{z,\infty}/(1 + q), \tag{16}
\]

\[
\langle m_z^2 \rangle_\infty = \vec{m}_{z,\infty}^2/(1 + q), \tag{17}
\]

\[
\langle m_z^4 \rangle_\infty = \vec{m}_{z,\infty}^4/(1 + q). \tag{18}
\]

3.3. Two-gaussian approximation for the magnetization distribution

Eqs. (13)-(18) describe the behavior of the system when we first set \( H = H^t \) and then take the limit \( L \to \infty \), but we also want to examine the leading corrections to the limiting behavior for large \( L \).

In pure phases, for large \( L \), we expect Gaussian distributions for the densities of extensive thermodynamic variables rather than \( \delta \)-functions [26]. For the uniform magnetization Gaussian distributions for the (scalar) quantity \( m_z \) in the two phases would give a distribution,

\[
P_L(m_z) \propto \frac{a_{AF}}{\sqrt{\chi_{zz}^{AF}}} \exp \left\{ - \frac{[m_z - (m_{z,\infty}^{AF} + \chi_{zz}^{AF} \Delta H)]^2}{2k_B T \chi_{zz}^{AF}/L^3} \right\} + \frac{a_{SF}}{\sqrt{\chi_{zz}^{SF}}} \exp \left\{ - \frac{[m_z - (m_{z,\infty}^{SF} + \chi_{zz}^{SF} \Delta H)]^2}{2k_B T \chi_{zz}^{SF}/L^3} \right\}, \tag{19}
\]

where \( a_{AF}, a_{SF} \) are constants determined by the ratios of the Gaussian amplitudes.
where 
\[ \Delta H = H - H^t. \]  
(20)
\[ \chi_{zz}^{SF}, \chi_{zz}^{AF} \] are the susceptibilities at \( H = H^t \) in the two phases, and \( a_{AF}, a_{SF} \) are the statistical weights of the two phases at \( H = H^t \). Further analysis shows that the susceptibility peak should scale as
\[ \chi_{zz}^{\text{max}} \approx \frac{\chi_{zz}^{AF} + \chi_{zz}^{SF}}{2} + \frac{(\Delta m)^2 L^3}{4k_B T}. \]  
(21)
Note that the location of this maximal magnetization fluctuation (i.e. susceptibility of the z-component of the uniform magnetization) occurs when the two weights are equal, i.e. \( a_{AF} = a_{SF} = 1/2 \). This condition readily yields \( q \exp(-\Delta F L^3/k_B T) = 1 \), i.e. \( \Delta F/k_B T = \ln q/L^3 \), or
\[ (H^{\text{max}} - H^t)/k_B T = -[\Delta m L^3]^{-1} \ln q. \]  
(22)
Since \( m_{z,\infty}^{AF} < m_{z,\infty}^{SF} \), the position of the susceptibility maximum relative to the transition point shifts to lower fields, \( H^{\text{max}} < H^t \), and scale with size like \( L^{-3} \).

The susceptibility at the transition point \( H^t \) is smaller by a factor \( 4q/(1+q)^2 \) than \( \chi_{zz}^{\text{max}} \) for \( L \rightarrow \infty \).

We remind the reader that for the weight for the low temperature phase of the Potts model, the factor \( q \) reflecting the degeneracy of the ordered phase is known, whereas here the value of a similar factor representing the difference in degeneracies of the SF and AF phases is unknown unless we rely on the hypothesis that \( q = \pi \).

4. Results
Monte Carlo simulations were performed at three different fixed temperatures \( T = 0.95J/k_B \), \( T = 0.80J/k_B \) and \( T = 0.60J/k_B \), all of which are below the bicritical point \( T_b \). The external field \( H \) was varied (using histogram reweighting) in order to determine the phase transition from AF to SF states. When not shown, error bars in the figures showing results are smaller than the size of the symbols.

The probability densities of the energy \( E \) per site are shown at the transition field \( H^t_L \) for different lattice sizes \( L \) in Fig. 4. For each \( L \) we chose the finite-size transition field to be at the point at which the (symmetric) peaks in the probability density for the energy were of equal heights.

For \( T = 0.95J/k_B \) (Fig. 4(a)), while the dip between the peaks was rather shallow for \( L = 40 \), it rapidly became quite deep for increasing values of \( L \) in agreement with the predictions of Binder [27] and Lee and Kosterlitz [28] for a first-order transition. For smaller values of \( L \) the probability density was almost flat, and the resultant thermodynamic properties showed such strong finite-size rounding that it was impossible to extract useful information about the
Figure 5. Extrapolation of the locations of the transition fields determined from the “equal height” rule for peaks in the probability distribution of the energy. (a) $T = 0.95 J/k_B$, (b) $T = 0.80 J/k_B$, (c) $T = 0.60 J/k_B$.

Table 1. Estimates for the latent heat $\Delta E$, the uniform magnetization change of the phase transition $\Delta m$, and the slope $dH^t/dT$ of the coexistence curve in the $H$-$T$ phase diagram by using the Clausius-Clapeyron relation and the one by using a B-spline interpolation at different temperature ($T = 0.95 J/k_B$, $0.80 J/k_B$, $0.60 J/k_B$).

| $T/(J/k_B)$ | $\Delta E$ | $\Delta m$ | $dH^t/dT$ (Eq. (23)) | $dH^t/dT$ (interpolation) |
|------------|------------|------------|---------------------|---------------------|
| 0.95       | 0.0250(7)  | 0.0352(4)  | 0.75(2)             | 0.78(3)             |
| 0.80       | 0.039(1)   | 0.092(1)   | 0.53(2)             | 0.54(2)             |
| 0.60       | 0.0271(8)  | 0.159(1)   | 0.28(1)             | 0.29(2)             |

The values of the transition field for each lattice size, $L$, as determined by the equal heights of the two peaks in the probability densities for the energy, are plotted in Fig. 5. Fig. 5(a) describes the case for $T = 0.95 J/k_B$. It shows very nicely that the variation is linear with $L^{-3}$ for $L \geq 40$. The estimated transition field in the thermodynamic limit is $H^t/J = 3.83830(5)$. Likewise, Fig. 5(b) corresponds to $T = 0.80 J/k_B$, and the transition field in the thermodynamic limit is estimated $H^t/J = 3.74053(6)$, by performing an extrapolation to $L = \infty$ for $L \geq 30$. Fig. 5(c) is for $T = 0.60 J/k_B$. Extrapolating to $L = \infty$ for $L \geq 24$, the transition field is $H^t/J = 3.65813(5)$.

By using the (magnetic) Clausius-Clapeyron relation, the slope $dH^t/dT$ of the coexistence curve in the $H$-$T$ phase diagram is given by [29],

$$dH^t/dT = \Delta E/(T \Delta m), \tag{23}$$

where $\Delta E$ is the latent heat and $\Delta m$ is the jump in uniform magnetization at the phase transition. Table 1 shows the estimates of the slope $dH^t/dT$ at different temperature ($T = 0.95 J/k_B$, $0.80 J/k_B$, $0.60 J/k_B$) obtained using the Clausius-Clapeyron relation. As $T$ decreases, $\Delta E$ first increases then decreases, while $\Delta m$ monotonically increases. With Eq. (23), the estimated slope $dH^t/dT$ monotonically decreases as $T$ decreases. The values of $dH^t/dT$ determined using a B-spline fit to the transition field values determined from the Monte Carlo simulations are shown for comparison. In all cases the agreement is excellent!

At $T = 0$, the transition field between SF and AF is $H^t/J = 3.6$ [11]. By applying a B-spline interpolation, we can also estimate the slope $dH^t/dT$, as shown in Table 1. The values of slope $dH^t/dT$ from the Clausius-Clapeyron relation and those from the interpolation agree with each
Fig. 6 shows the $H$-$T$ phase diagram for the 3D anisotropic Heisenberg model in an external field, where the dashed curve is a B-spline interpolation.

The probability distributions of the SF order parameter $\psi$ at $T = 0.95 J/k_B$, $T = 0.80 J/k_B$, and $T = 0.60 J/k_B$ are shown at the transition field for different lattice sizes $L$ in Fig. 7. For each size we chose the finite size transition field to be located at the same point at which the (symmetric) peaks in the probability distribution for the energy were of equal heights. These data show that the distributions contain two clear peaks at $\pm \psi_\infty$ corresponding to the SF order and a peak centered about zero corresponding to the AF phase. These peaks cannot be described solely by Gaussians since the states describing phase coexistence (from about $|\vec{\psi}| \approx 0.2$ to $|\vec{\psi}| \approx 0.36$ at $T = 0.95 J/k_B$) are not yet strongly suppressed. If we “separate” the distributions into two peaks by choosing the minimum probability as the separation point, we can measure the “weight” of each peak by numerically integrating the probability under each peak. As shown in Table 2 the relative weight of the sum of the “ordering” peaks and the disordered peak depends upon the exact choice of $H^t$ and is also slightly dependent upon the choice of $L$. For our best estimate of $H^t/J = 3.838305$ at $T = 0.95 J/k_B$, the value appears to be converging for large $L$ to the estimate of $q = \pi$ that was obtained earlier using the two Gaussian approximation. Similar behavior happens at the best estimates for $H^t/J$ for $T = 0.80 J/k_B$ and $T = 0.60 J/k_B$ as well. We remind the reader that the result $q = \pi$ was already predicted from
Table 2. Estimates for $q_{\text{eff}}$ from the ratio of probability distributions of the weights of the peaks for different values of $L$. (Top) $T = 0.95J/k_B$, (Middle) $T = 0.80J/k_B$, (Bottom) $T = 0.60J/k_B$.

| $L$ | $H^f/J = 3.838300$ | $H^f/J = 3.838305$ | $H^f/J = 3.838310$ |
|-----|-------------------|-------------------|-------------------|
| 60  | 3.31(23)          | 3.42(30)          | 3.53(28)          |
| 80  | 3.15(24)          | 3.36(26)          | 3.75(29)          |
| 100 | 2.82(30)          | 3.19(29)          | 3.82(30)          |

| $L$ | $H^f/J = 3.740520$ | $H^f/J = 3.740525$ | $H^f/J = 3.7405230$ |
|-----|-------------------|-------------------|-------------------|
| 40  | 3.16(23)          | 3.27(25)          | 3.38(21)          |
| 50  | 3.06(33)          | 3.28(27)          | 3.51(31)          |
| 60  | 2.86(24)          | 3.23(26)          | 3.66(30)          |

| $L$ | $H^f/J = 3.658125$ | $H^f/J = 3.658130$ | $H^f/J = 3.658135$ |
|-----|-------------------|-------------------|-------------------|
| 28  | 3.30(21)          | 3.39(23)          | 3.48(26)          |
| 32  | 3.22(26)          | 3.36(30)          | 3.51(31)          |
| 40  | 3.04(24)          | 3.31(28)          | 3.62(31)          |

Table 3. The ratios of first and second moments of $\psi$, $\tilde{m}_z$ at the transition field $H^t$ at different temperature ($T = 0.95J/k_B, 0.80J/k_B, 0.60J/k_B$).

| $T/(J/k_B)$ | $\langle|\psi|\rangle_L|_{H^t}/\psi_\infty$ | $\langle\psi^2\rangle_L|_{H^t}\psi^2_\infty$ | $\langle|\tilde{m}_z|\rangle_L|_{H^t}\tilde{m}_z,\infty$ | $\langle\tilde{m}_z^2\rangle_L|_{H^t}\tilde{m}_z^2,\infty$ |
|-------------|------------------------------------------|---------------------------------------------|---------------------------------------------|---------------------------------------------|
| 0.95        | 0.77(3)                                 | 0.74(3)                                    | 0.32(4)                                    | 0.26(3)                                    |
| 0.80        | 0.78(3)                                 | 0.75(4)                                    | 0.30(4)                                    | 0.24(3)                                    |
| 0.60        | 0.78(4)                                 | 0.76(3)                                    | 0.29(4)                                    | 0.25(3)                                    |

the two delta-function distribution appropriate to the thermodynamic limit in Eq. (10).

One of the most striking results of our study emanates from Eqs. (13), (14), (16), and (17). Plots of $\langle|\psi|\rangle_L$, $\langle\psi^2\rangle_L$, $\langle|\tilde{m}_z|\rangle_L$, and $\langle\tilde{m}_z^2\rangle_L$, vs $H$ should show common intersection points for different $L$ at $H^t$. These features would not occur at a second-order transition, but are quite consistent with our phenomenological theory. From Eqs. (13) and (14) we conclude that

$$\frac{\langle|\psi|\rangle_L}_{|\psi_\infty|} = \frac{\langle\psi^2\rangle_L}{\psi^2_\infty} = \frac{q}{1+q} \approx 0.7585 \quad (24)$$

and from Eqs. (16) and (17)

$$\frac{\langle|\tilde{m}_z|\rangle_L}_{\tilde{m}_z,\infty} = \frac{\langle\tilde{m}_z^2\rangle_L}{\tilde{m}_z^2,\infty} = \frac{1}{1+q} \approx 0.2415 \quad (25)$$

The simulation data show small but systematic shifts with increasing system size and we can only say that the predictions are consistent with the current data, which are shown in Table 3. These values are in quite reasonable agreement with predictions although more precise values would be needed to draw strong conclusions. However, the discrepancies between the measured and predicted values noted above can probably be attributed to the difference in the location of the intersections and our best estimate for the transition field in the thermodynamic limit.
Using more precise data on still larger systems to extrapolate the small finite size variations to $L \to \infty$ could give slightly different estimates than quoted above but would require prohibitively large resources at the present time.

5. Conclusion

The finite-size behavior of a first-order transition from a state with simple, discrete degeneracy to a state with an infinite degeneracy was explored using a combination of phenomenological theory and Monte Carlo simulations to study the antiferromagnetic to spin-flop state transition in a uniaxially anisotropic Heisenberg antiferromagnet on $L^3$ simple cubic lattices in an external field $H$ applied along the easy axis.

The phenomenological theory was based upon phase coexistence in the thermodynamic limit with probability distributions of the system in each phase described by delta functions. We conjectured that the relative weights of the AF and SF phases are 2 and $2\pi$ by integrating over the angle $\phi$ of the two-component SF order parameter. This implies an “effective” relative degeneracy $q = \pi$ with no adjustable parameters.

The finite-size behavior of the model was determined using high resolution Monte Carlo simulations. The phase transition was located precisely using an equal height rule for the probability distribution for the internal energy as well as via crossing points of moments and cumulants. Different predictions from the theory yield consistent values for the effective value of the degeneracy $q$ for sufficiently large values of $L$. Simulations were performed at three different temperatures along the spin-flop boundary, and in all cases we found quantitatively consistent results and $q = \pi$.

We, therefore, conclude that the simple theory based upon a double Gaussian distribution correctly describes the finite-size effects at first-order transitions between phases with different symmetries of the order parameters. Most importantly, the underlying theory does not depend on the fine details of the model; hence a new kind of universality at a first-order transition has been identified.

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References

[1] Fisher M E 1971 Critical Phenomena ed Green M S (New York: Academic Press) pp 1–98
[2] Privman V 1990 Finite Size Scaling And Numerical Simulation Of Statistical Systems (Singapore: World Scientific)
[3] Landau D P 1976 Phys. Rev. B 13(7) 2997–3011
[4] Binder K and Landau D P 1984 Phys. Rev. B 30(3) 1477–1485
[5] Borgs C and Kotecký R 1990 J. Stat. Phys. 61 79–119 ISSN 1572-9613
[6] Challa M S S, Landau D P and Binder K 1986 Phys. Rev. B 34(3) 1841–1852
[7] Landau D P and Binder K 2015 A Guide to Monte Carlo Simulations in Statistical Physics 4th ed (Cambridge: Cambridge University Press)
[8] Fisher M E 1975 AIP Conf. Proc. 24 273
[9] Nelson D R, Kosterlitz J M and Fisher M E 1974 Phys. Rev. Lett. 33(14) 813–817
[10] Kosterlitz J M, Nelson D R and Fisher M E 1976 Phys. Rev. B 13(1) 412–432
[11] Landau D P and Binder K 1978 Phys. Rev. B 17(5) 2328–2342
[12] Mouritsen O G, Hansen E K and Jensen S J K 1980 Phys. Rev. B 22(7) 3256–3270
[13] Calabrese P, Pelissetto A and Vicari E 2003 Phys. Rev. B 67(5) 054505
[14] Folk R, Holovatch Y and Moser G 2008 Phys. Rev. E 78(4) 041124
[15] Bannasch G and Selke W 2009 Eur. Phys. J. B 69 439–444 ISSN 1434-6036
[16] Selke W 2011 Phys. Rev. E 83(4) 042102
[17] Hu S, Tsai S H and Landau D P 2014 Phys. Rev. E 89(3) 032118
[18] Xu J, Tsai S H, Landau D P and Binder K 2019 Phys. Rev. E 99(2) 023309
[19] Fisher M E and Nelson D R 1974 Phys. Rev. Lett. 32(24) 1350–1353
[20] Gorter C J and Van Peski-Tinbergen T 1956 Physica 22 273
[21] Metropolis N, Rosenbluth A W, Rosenbluth M N, Teller A H and Teller E 1953 J. Chem. Phys. 21 1087
[22] Berg B A and Neuhaus T 1992 Phys. Rev. Lett. 68(1) 9–12
[23] Ferrenberg A M and Swendsen R H 1988 Phys. Rev. Lett. 61 2635
[24] Potts R B 1952 Math Proc. Cambridge 48 106109
[25] Wu F Y 1982 Rev. Mod. Phys. 54(1) 235–268
[26] Landau L D and Lifshitz E M 1980 Statistical Physics 3rd ed (Amsterdam: Elsevier)
[27] Binder K 1982 Phys. Rev. A 25(3) 1699–1709
[28] Lee J and Kosterlitz J M 1990 Phys. Rev. Lett. 65(2) 137–140
[29] Callen H 1985 Thermodynamics and an Introduction to Thermostatistics 2nd ed (New York: Wiley)