Location of the Bicritical Point of the Anisotropic Heisenberg Model in a Crystal Field

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Abstract. Extensive Monte Carlo simulations are used to locate the bicritical point of the ferromagnetic anisotropic Heisenberg model on a simple cubic lattice in the presence of a crystal field. In order to achieve this goal, we employ a hybrid algorithm comprising Metropolis and Wolff algorithms along with field mixing. Multiple histogram techniques have also been used to obtain the probability distribution function of the conjugate extensive variables of interest. In conjunction with finite-size scaling analysis we computed the fourth-order cumulant of the order parameter along the first-order line and the corresponding bicritical point has been located from the crossings of the cumulants.

1. INTRODUCTION

In a recent paper [1], Plascak and Martins review the importance of the order parameter probability distribution to investigate the critical properties and locate multicritical points through Monte Carlo simulations in statistical mechanics models, in particular discrete state models. This tool has been successfully employed along with field mixing techniques to locate multicritical points, for example the double critical end point of the two-dimensional spin-3/2 Blume-Capel model [2], the tricritical point of a two-dimensional spin fluid [3], the asymmetric Ising model [4], the two-dimensional Potts model [5], the three-dimensional XXZ model [6], among others. In particular, we have already used this technique to locate the tricritical point of the XY vector Blume-Emery-Griffiths model in three dimensions [7]. Here we once again apply this technique to study a continuous spin model.

In a previous work [8] we have investigated, through Monte Carlo simulations [9], the phase diagram of the anisotropic ferromagnetic Heisenberg model in a crystal field on a simple cubic lattice, which reveals a rich topology due to the competition between crystalline and exchange anisotropies. This phase diagram, depicted in Fig. 1 for a finite lattice of linear size $L = 14$, shows two ordered phases, separated by a first-order transition line. The Ising-like ordered phase has an easy axis ordering (z axis), while the XY-like phase has an easy plane ordering, perpendicular to the z axis. Each ordered phase is separated from the disordered paramagnetic

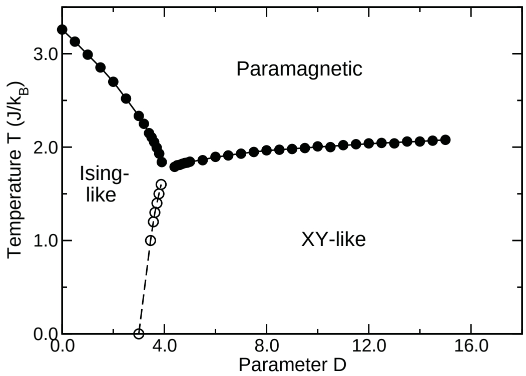

Figure 1. Phase diagram for the anisotropic Heisenberg model in a crystal field on a simple cubic lattice (L=14). Lines are only guide to the eyes. The continuous lines and full circles indicate second-order phase transitions, while the dashed line and open circles stand for first order phase transitions. As mentioned in [8], the finite-size scaling behavior performed revealed that the extrapolated temperatures were very close (less than 1% discrepant) to those obtained by taking L=14, justifying, for our purposes, the use of such lattice size to obtain the phase diagram. Error bars are of the size or smaller than symbol sizes.

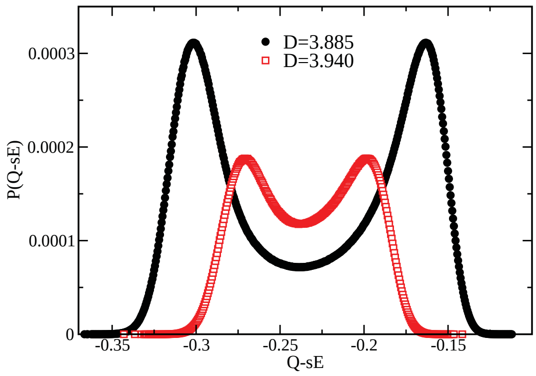

Figure 2. Probability distribution function for the field mixing extensive conjugate variable $\mathcal{Q} = Q - sE$ (L=20). The distribution displayed refers to two different points along the first-order line. Error bars are of the size or smaller than symbol sizes.

phase by a second-order transition line. All transition lines terminate at a bicritical point. It is the location of this bicritical point that we want now to determine with better precision.

The model is defined by the hamiltonian

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} (\vec{S}_i \cdot \vec{S}_j) - A \sum_{\langle i,j \rangle} S_i^z S_j^z + D \sum_{i=1}^{N} (S_i^z)^2, \tag{1}$$

where $\vec{S}$ stands for a classical three dimensional spin vector with unity modulus and $\langle i,j \rangle$ stands for a sum over first-neighbor spins on an N spin simple cubic lattice. J is the ferromagnetic ($J = 1$) exchange interaction parameter, A refers to the easy-axis exchange anisotropy ($A > 0$) and D is related to the easy-plane crystalline interaction (we consider herein $D > 0$). In this work we used $A = 1$.

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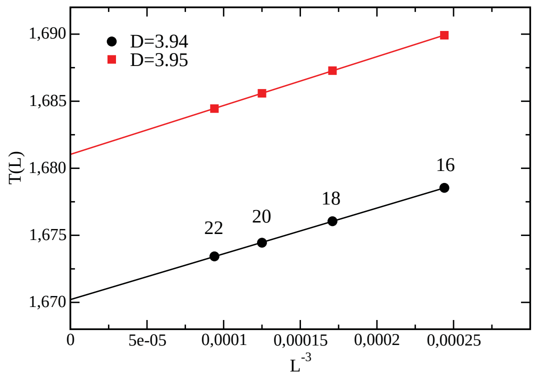

Figure 3. Finite size scaling analysis for two different points along the first-order line. The line is the best fit to the data points for the indicated lattice sizes. Error bars are smaller than symbol sizes.

2. RESULTS

Simulations were performed on a simple cubic lattice with L=16, 18, 20 and 22. In order to reduce critical slowing down, we used a hybrid Monte Carlo scheme [10], performing four Wolff [11] steps after one Metropolis [12] sweep. The Wolff algorithm was adapted to take into account the anisotropies and dimensionality of the model based on the scheme proposed in Ref. [13]. In order to achieve good precision we had to perform very long runs (ranging from 280 to 690 million hybrid Monte Carlo steps).

Using field mixture [1, 14] and multiple histogram techniques [9, 15, 16, 17], we probed the probability distribution of the conjugate extensive variable associated with the parameters D and T in order to precisely locate the first-order transition line. This was achieved tuning the values of the mixing parameter s and temperature T for a given value of the parameter D and a specific lattice size L in order to obtain a symmetric distribution, as shown in Fig. 2 for two values of the parameter D. Having the finite-size pseudo-transition temperature for each lattice size, we performed the finite-size scaling analysis and determined the transition temperature. In Fig. 3, the finite size scaling analysis is shown for two different values of the parameter D along

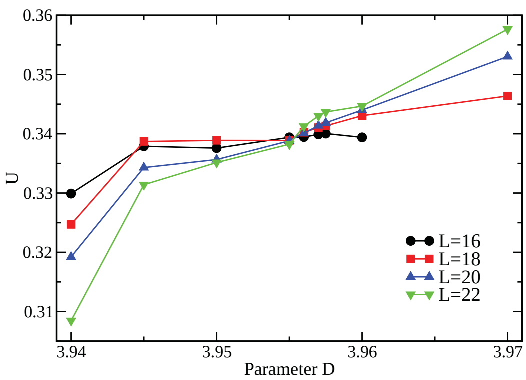

Figure 4. Fourth-order cumulant of the order parameter for the three-dimensional anisotropic Heisenberg model. Lines are only guide to the eyes and the error bars are smaller than the symbol sizes.

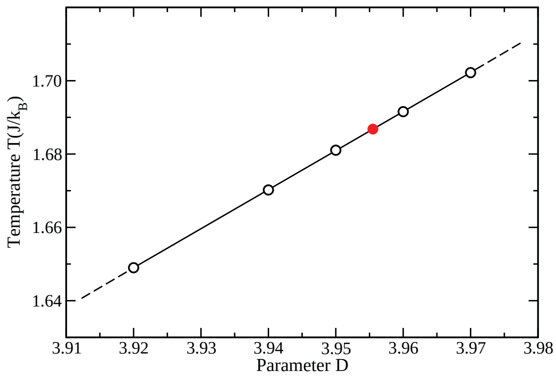

Figure 5. First-order transition line and its analytical extension on the $D-T$ plane, obtained with the procedure described in the text. The bicritical point is depicted in red. Lines are only guide to the eyes and the error bars are smaller than the symbol sizes.

the first-order line. The conjugate extensive variable of interest here is $\mathcal{Q} = Q - sE$, where

$$Q = \sum_{i=1}^{N} (S_i^z)^2, \tag{2}$$

and

$$E = \sum_{\langle i,j \rangle} (\vec{S}_i \cdot \vec{S}_j). \tag{3}$$

We then computed the fourth-order cumulant of the order parameter (the z-component of the magnetization) along the first-order line, defined as

$$U = 1 - \frac{\langle m_z^4 \rangle}{3 \langle m_z^2 \rangle^2}, \tag{4}$$

where

$$m_z = \sum_{i=1}^{N} S_i^z. \tag{5}$$

At the bicritical point, the fourth-order cumulant should coincide for sufficiently large system sizes. Thus, following the first-order transition line, we searched the cumulant crossing in order to determine the bicritical point.

According to the cumulant crossing (Fig. 4), the bicritical point was located at $D = 3.9555(4)$, which corresponds to a bicritical temperature $T = 1.6868(4)$. In Fig. 5, the first-order transition line is depicted, along with its analytical extension, whose beginning is marked off by the bicritical point.

3. CONCLUSIONS

In summary, employing field mixing and multiple histogram techniques, we have located the bicritical point of the three-dimensional anisotropic Heisenberg model with very good precision at $D = 3.9555(4)$ and $T = 1.6868(4)$. Further results concerning the bicritical behavior of this model will be published elsewhere.

4. ACKNOWLEDGMENTS

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