Dynamic critical behavior of the classical anisotropic BCC Heisenberg antiferromagnet

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Using a recently implemented integration method [Krech et al.] based on an iterative second-order Suzuki-Trotter decomposition scheme, we have performed spin dynamics simulations to study the critical dynamics of the BCC Heisenberg antiferromagnet with uniaxial anisotropy. This technique allowed us to probe the narrow asymptotic critical region of the model and estimate the dynamic critical exponent $z = 2.25 \pm 0.08$. Comparisons with competing theories and experimental results are presented.

I. INTRODUCTION

Despite their relative simplicity, classical Heisenberg models can be used to describe the dynamic critical behavior of magnetic materials whose ions have large effective spin values. For example, RbMnF$_3$ is well modeled by an isotropic Heisenberg antiferromagnet, whereas MnF$_2$ and FeF$_2$ are good physical realizations of the Heisenberg antiferromagnet with weak and strong uniaxial anisotropies, respectively.

The effect of uniaxial anisotropy on the critical dynamics has been the subject of many theoretical and experimental studies. Although both indicate that the dynamic structure factor has a dominant purely transverse component and a suppressed propagative transverse component, there is still controversy about the dynamic critical exponent $z$. While a dynamic scaling argument and mode-coupling theory indicate that $z = 2$, a combination of renormalization group theory and $\epsilon$-expansion predicts that $z = 2 + \alpha/\nu$. Using the Ising value $\nu = 0.6289(8)$ from a high resolution Monte Carlo study and $\alpha = 0.110(5)$ from field theory [2], the latter prediction is $z = 2.175(10)$. Experiments on FeF$_2$ have not had enough resolution to distinguish between these two predictions, and on MnF$_2$ the exponent obtained was that of the isotropic antiferromagnet, $z = 1.5$. Presumably this very low value is due to crossover effects resulting from the weak anisotropy in MnF$_2$.

Our approach to this problem is to use spin dynamics simulations with an efficient integration scheme. The dynamic critical exponent is estimated using a dynamic finite-size scaling theory and compared with the predictions by the different theories and with experiments.

II. MODEL AND METHODS

The Hamiltonian of the model is given by

$$H = J \sum_{<\mathbf{r},\mathbf{r}'>} \mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}'} - D \sum_{\mathbf{r}} \langle S_{\mathbf{r}}^z \rangle^2$$

(1)

where $\mathbf{S}_{\mathbf{r}} = (S_{\mathbf{r}}^x, S_{\mathbf{r}}^y, S_{\mathbf{r}}^z)$ is a three-dimensional classical spin of unit length, $<\mathbf{r},\mathbf{r}'>$ denotes nearest-neighbor pairs of spins coupled by the antiferromagnetic exchange interaction $J > 0$, and $D$ is the uniaxial single-site anisotropy. We use $D = 0.0591J$ and the inverse critical temperature $1/T_c = 0.478k_B/J$ appropriate for MnF$_2$. We consider body-centered-cubic lattices with linear sizes $12 \leq L \leq 60$, corresponding to $2L^3$ sites, and periodic boundary conditions.

The time evolution of the spins is governed by coupled equations of motion, and the dynamic structure factor $S(q,\omega)$, for momentum transfer $q$ and frequency $\omega$, observable in neutron scattering experiments, is the Fourier transform of the space-displaced, time-displaced spin-spin correlation function $C^K(r - r', t)$, defined as

$$C^K(r - r', t) = \langle S^K(t)S^K(0) \rangle - \langle S^K(t) \rangle \langle S^K(0) \rangle$$

with $K = x, y, z$. Because of the periodic boundary conditions, we can only access a set of discrete values of momentum transfer given by $q = 2\pi n_q/L$, where $n_q = \pm 1, \pm 2, ..., \pm L/2$.

Equilibrium configurations at $T_c$ were generated using a hybrid Monte Carlo method where each hybrid step consisted of two Metropolis sweeps through the lattice and eight Wolff cluster spin flips. Typically 3000 hybrid Monte Carlo steps were used to generate each equilibrium configuration, which was then used as an initial spin configuration in the integration of the coupled equations of motion. We use 2040 initial configurations to compute the averages. For the largest lattice used ($L = 60$), there are 432,000 coupled equations to integrate. These numerical integrations were performed to a maximum time of $t_{max} = 400/J$, using an iterative second-order Suzuki-Trotter decomposition method implemented by Krech et al., with two iterations and a time step of $\delta t = 0.04/J$. This method consists of performing explicit rotations of a spin about its local effective field. The lattice is divided into two sublattices $A$ and $B$, and a formal solution of the equations of motion yields $y(t + \delta t) = e^{(A+B)\delta t}y(t)$, where $y = (y_A, y_B)$ denotes collectively all the spins, and the matrices $A$ and $B$ are the infinitesimal generators of rotation of the spin configurations $y_A$ on sublattice $A$ at fixed $y_B$ and of the spin configurations $y_B$ on $B$ at fixed $y_A$, respectively. The spin configurations on sublattices $A$ and $B$ are updated in succession, using the second-order Suzuki-Trotter decomposition of the exponential operator $e^{(A+B)\delta t}$, given by $e^{(A+B)\delta t} = e^{A\delta t/2}e^{B\delta t}e^{A\delta t/2} + O(\delta t^3)$. A
similar scheme using a fourth-order decomposition of the exponential operator has also been tested in Ref. 9. The iterative procedure is necessary because of the single-site anisotropy.

The finite integration time introduces oscillations when the Fourier transform of \( C^k(x - x', t) \) is taken to produce \( S(q, \omega) \) and we smooth them out by convoluting the spin-spin correlation function with a Gaussian resolution function in frequency, with characteristic width \( \delta_\omega \).

The dynamic structure factor thus obtained is denoted as \( S^k(q, \omega) \).

The dynamic critical exponent \( z \) can be determined from dynamic finite-size relations [11], given by

\[
\omega^k S^k(q, \omega) / \chi_k^z(q) = G(\omega L^z, qL, \delta_\omega L^z)
\]

where \( \chi_k^z(q) = \int_{-\infty}^{\infty} S^k(q, \omega) d\omega / 2\pi \) is the momentum dependent susceptibility and \( \omega_m \) is a characteristic frequency, given by \( \int_{-\omega_m}^{\omega_m} S^k(q, \omega) d\omega / 2\pi = \chi_k^z(q)/2 \). To estimate \( z \) we choose the width of the resolution function to be \( \delta_\omega = 0.015(60/L)^z \) so that the function \( \Omega(qL, \delta_\omega L^z) \) in Eq. (2) is constant if \( qL \) is fixed, yielding

\[
\omega_m \sim L^{-z}.
\]

Because \( \delta_\omega \) depends on \( z \), this exponent had to be determined iteratively. The coefficient 0.015 of \( \delta_\omega \) was chosen empirically as a compromise between effectively reducing the oscillations in \( S(q, \omega) \) and not excessively broadening its structure.

III. RESULTS AND DISCUSSION

Our simulations, performed at the critical temperature for MnF\(_2\), show that while the transverse component \( S^T(q, t) \) of the space-Fourier-transformed correlation function \( S(q, t) \) has a short relaxation time, the longitudinal component \( S^z(q, t) \) decays extremely slowly [see Fig. (1)], and this requires that the equations of motion be integrated to very long times. Although our \( t_{\max} \) is still not large enough for the longitudinal component to decay to a value that is close to zero, it is a significant improvement over the maximum time we could reach with more standard integration methods, such as the fourth-order predictor-corrector method, with our current computing resources. Whenever not shown, error bars are smaller than the symbol sizes in the figures.

The longitudinal component of the dynamic structure factor, \( S^z(q, \omega) \), shown in Fig. (2a), has a purely dissipative behavior, as indicated by the single central peak. In contrast, the transverse component \( S^T(q, \omega) \) contains a propagative mode, indicated by the spin wave peak in Fig. (2b), with a possible small central peak as well. A comparison between Figs. (2a) and (2b) shows that the longitudinal component has a much larger intensity. The dispersion curve \( \omega(q) \) of the spin waves along the [100] direction is shown in Fig. (3), where the solid line represents a fit to the function \( \omega = \omega_0 + cq^2 \). The non-zero value of the frequency in the limit as \( q \to 0 \) is characteristic of an anisotropic model. These results for the dynamic structure factor are in qualitative agreement with theory and experimental results.

An estimate for the dynamic critical exponent \( z \) was
obtained iteratively using Eq. (3) for different values of \( n_q \). Such estimates are denoted as \( z_q \) and are shown in Fig. 4. For the weakly anisotropic system considered here, the onset of the asymptotic critical region occurs at very low values of \( q \), accessible only with very large lattice sizes (and not accessible to experiments yet). Therefore, a better estimate for \( z \) is given by \( z_0 \), obtained by extrapolating \( z_q \) to the limit \( q \to 0 \). We fitted \( z_q \) with the function \( z_q = z_0 + a n_q + b n_q^c \), using \( n_q = 1, 2, ..., n_q^{\text{max}} \), where \( z_0, a, b, \) and \( c \) are fitting parameters. To check the robustness of the extrapolated \( z_0 \), we have also performed fittings with fixed \( c = 2 \). The systematic change in the value of \( z_0 \) for both types of fittings was studied as the number of points included in the fittings increased, from \( n_q^{\text{max}} = 4 \) and 5, for the fittings with \( c = 2 \) and variable \( c \), respectively, to \( n_q^{\text{max}} = 15 \). For \( n_q^{\text{max}} \) up to 7, the \( \chi^2 \) of the fittings is reasonable, and there is no clear systematic change in the value of \( z_0 \); hence, the average \( z_0 \) from these fittings yields \( z = 2.25 \pm 0.08 \), which is the first numerical estimate of the dynamic critical exponent for this model.

IV. SUMMARY AND CONCLUSIONS

Because of difficulties for experiments to probe the critical region, experimental data have not yet been able to distinguish between competing theories. While limited by finite lattice size and finite integration time, simulations offer the hope of shedding light on the differences between theories and experiment. Although not yet conclusive, our estimate of \( z = 2.25 \pm 0.08 \) is slightly larger than, but consistent with, the prediction by the renormalization group theory. It is not consistent with mode-coupling theory and the dynamic scaling prediction.

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