Spin dynamics calculations in the two-dimensional classical XY-model [1]

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Abstract. We report preliminary results from the first large scale numerical study of critical spin dynamics in the two dimensional classical XY model. We integrate the hamiltonian equations of motion, starting from a set of configurations generated by Monte Carlo. In addition to the expected spin wave peak in the Kosterlitz-Thouless phase, we find a strong central peak, and unexpected structure below the spin wave peak. The dynamic critical exponent is measured to be $z = 1.00(4)$ in the KT-phase.

1 Introduction

We have investigated the dynamic critical behavior of the two-dimensional classical anisotropic Heisenberg model (XY-model)

$$\mathcal{H} = -J \sum_{nn} \left(\mathbf{S}_i^x \mathbf{S}_j^x + \mathbf{S}_i^y \mathbf{S}_j^y + \lambda \mathbf{S}_i^z \mathbf{S}_j^z \right) \ , \lambda \equiv 0 \, . \tag{1}$$

The statics of this model are similar to those of the "plane rotator model", i.e. the model with *two*-component spins: at all temperatures $T \leq T_{KT}$ the model is in a Kosterlitz-Thouless phase [1], where it is dominated by vortex-pairs, does not have long range order, and is *critical*, with static correlations decaying like $\langle S(0)S(r) \rangle \sim r^{-\eta}$. The static critical exponent η is 1/4 at T_{KT}. Above T_{KT}, vortices unbind and the correlations decay exponentially.

The *dynamics*, however, are very different: The XY-model possesses equations of motion

$$\frac{d}{dt}\mathbf{S}_i = \mathbf{S}_i \times \left[-J \sum_{nn} \left(\mathbf{S}_j^x \hat{\mathbf{e}}_x + \mathbf{S}_j^y \hat{\mathbf{e}}_y \right) \right] , \tag{2}$$

where $\hat{\mathbf{e}}_x$ and $\hat{\mathbf{e}}_y$ are unit vectors in the x- and y-directions respectively. Eq. (2) is a set of coupled equations and can be integrated numerically. The plane rotator model, on the other hand, does not possess hamiltonian equations of motion; there is only relaxational dynamics.

To obtain the dynamic critical behavior for each temperature, we generated a set of equilibrium configurations by Monte Carlo simulations and

[1] 'Computer Simulations in Condensed Matter Physics VIII", ed. D.P. Landau et al., Springer Proceedings in Physics, 1995, p.175

integrated the hamiltonian equations of motion for each configuration up to a maximum time t_{max}. For each time evolution, we measured the time-displaced, space-displaced spin-spin correlation function. The time- and space-fourier transform of this function is the dynamic structure factor (neutron scattering function) $S(q, \omega)$.

In the present paper we emphasize several technical aspects of our study, as well as an unexpected structure observed in $S(q, \omega)$. We will present a detailed physical discussion of $S(q, \omega)$ elsewhere [2]. An earlier exploratory study [3] indicated a rich structure in the neutron scattering function which was not adequately described by theory.

2 Simulations and Time Integration

Most of our simulations were performed below T_{KT}, where the system is critical. The spatial correlation length there is only limited by the system size. Standard Monte Carlo procedures will therefore suffer from severe Critical Slowing Down. In order to reduce autocorrelations we employed a hybrid method in which each update consisted of 2 fully vectorized checkerboard Metropolis updates, 8 Overrelaxation updates [4], and one Single-Cluster update [5]. In the overrelaxation algorithm [4] each spin is reflected with respect to a plane, in such a way that its contribution to the total energy remains constant. The spin z-component is not changed during this update. The algorithm is vectorized in checkerboard fashion. The cluster algorithm is also restricted to changes in the xy-plane. A single cluster is constructed, in complete analogy with Wolff's cluster algorithm [5] for the plane rotator model. Since both overrelaxation and Cluster updates leave the z-components of spins unchanged, Metropolis updates are necessary to ensure ergodicity. Inclusion of the cluster updates reduced autocorrelations drastically, e.g. at $T = 0.6$, $L = 128$, from about 300 hybrid sweeps when omitting the cluster updates down to about 3 hybrid sweeps.

We generated between 500 and 1200 independent spin-configurations for each combination of temperatures $T = 0.4$, 0.6, $0.725 \approx T_{KT}$, $T = 0.8$ and lattice sizes from 16^2 to 192^2, with about 200 hybrid sweeps between configurations. We found this many configurations to be necessary in order to sufficiently reduce thermal fluctuations in the resulting neutron scattering function. The error bars in our figures represent the statistical errors for averages over the equilibrium configurations.

Starting with each equilibrium configuration, the time dependence of the spins was determined from the coupled set of equations of motion, eq. (2), which was integrated numerically using a vectorized fourth order predictor-corrector method [6], with a time step size of $\delta t = 0.01 J^{-1}$. This method has a very small systematical error, of order $(\delta t)^5$. The maximum integration time was $t_{max} = 400 J^{-1}$. (A few runs were also performed for lattice size

256^2 with $t_{max} = 800J^{-1}$ and produced the same physical results.) We chose a very large t_{max} in order to sufficiently reduce cutoff effects in $S(q,\omega)$, as discussed below. This value of t_{max} is much larger than any employed in previous studies, and the time integration could potentially become unstable. We checked stability by verifying that $S(q,\omega)$ remained unchanged when we introduced an *additional* time integration of length $200J^{-1}$ before starting to measure space-time correlation functions. In addition, we found that the total energy changed by a relative factor of less than 3×10^{-6} between $t = 0$ and t_{max}.

3 Extracting $S(q,\omega)$

In order to determine $S(q,\omega)$, we measured the space displaced, time displaced spin-spin correlation function $C^{kk}(\mathbf{r}-\mathbf{r}', t-t') = \left\langle S^k_{\mathbf{r}}(t) S^k_{\mathbf{r}'}(t')\right\rangle$ for each time evolution, with $t - t' \le t_{cut} \equiv 0.9\, t_{max}$, and averaged results over the different time evolutions, and over $t \in \{0, t_{max}/10\}$. Fourier transforms in space and time then gave $S^{kk}(\vec{q},\omega)$. Spatial xy symmetry allows averaging over S^{xx} and S^{yy}. We saved a large amount of storage space by fixing the direction of $\vec{q}$ to $(q,0)$ or $(0,q)$, and averaging over the results. Since $S(q,\omega)$ is a convolution, it can be computed efficiently by use of Fast Fourier Transforms, which saved a large amount of CPU time.

Note that a temporal fourier transform with a finite time cutoff t_{cut} produces *oscillations* in $S(q,\omega)$, with period $2\pi/t_{cut}$. These oscillations hinder analysis of $S(q,\omega)$, for example at the very narrow spin wave peak. To reduce the impact of the cutoff, one can *smoothen* $S(q,\omega)$ by multiplying the correlation function with a damping factor, e.g. $\exp(-\frac{1}{2}(t\,\delta\omega)^2)$. Smoothening widens all features in $S(q,\omega)$, similar to the effect of finite ω-resolution in an experiment. It also complicates analysis of the data by Dynamic Finite Size Scaling [6].

Fig. 1 shows an example of $S(q,\omega)$ with different values of t_{max}. For small $t_{max} = 100J^{-1}$, oscillations are strong, and the spin wave peak is too broad. A damping factor of $\delta\omega = 0.02$ smoothens the oscillations, but it also further broadens the peak. Both oscillations and broadening are overcome by integrating up to $t_{max} = 400J^{-1}$. For critical dynamics, larger lattice sizes necessitate larger integration times. We found dynamic finite size scaling to be a very sensitive tool to determine which values of t_{max} are sufficient [2].

4 Results

We summarize briefly the main conclusions from a first analysis of our data. Detailed results will be presented elsewhere [2].

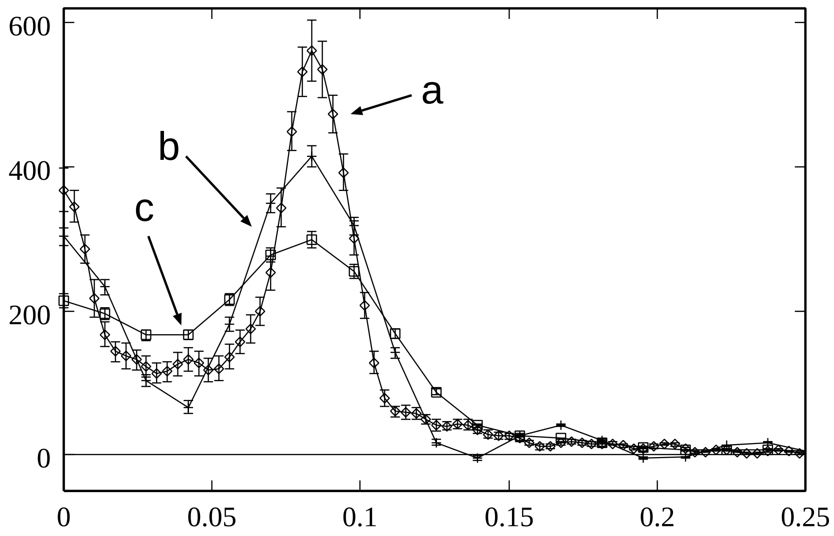

Figure 1: $S^{xx}(q,\omega)$ at $T = 0.725$, $L = 192$, $q = 2 \times \frac{2\pi}{L}$, with (a) $t_{max} = 400$, $\delta\omega = 0$, (b) $t_{max} = 100$, $\delta\omega = 0$, and (c) $t_{max} = 100$, $\delta\omega = 0.02$.

The two main physical features in $S(q,\omega)$ are the spin wave peak and an unexpectedly large central peak around $\omega = 0$. The spin wave peak is present in S^{xx} at all temperatures $T \leq T_{KT}$; above T_{KT} there is only a large central peak. As T increases, the spin wave peak in S^{xx} becomes wider and moves to smaller ω; with increasing q it becomes wider and weaker. Its shape is not well described by existing theoretical calculations [7]. There is a sizeable central peak in S^{xx} even at $T \leq T_{KT}$, which was not predicted. It becomes wider and stronger with increasing T. The out-of-plane correlations S^{zz} also show a weak and rather sharp spin wave peak at all temperatures. It is wider than the predicted delta function [7] would produce with our finite integration time. The dispersion relation (position of the spin wave peak versus momentum) is linear at small q for $T \leq T_{KT}$, and nonlinear above T_{KT}, as expected.

By dynamic finite size scaling [2] we determined the dynamic critical exponent z. Both a characteristic frequency ω_m and $S(q,\omega)$ itself scale very well, and we obtained $z = 1.00(4)$ for all $T \leq T_{KT}$, in agreement with theoretical predictions [7].

In addition to the spin wave peak and central peak, there is additional unexpected structure in S^{xx}, namely several smaller peaks at multiples of a basic frequency ω_b. An example is shown in fig. 2. Note that the logarithmic scale strongly overemphasizes the additional peaks. The positions of these peaks coincide with the positions of spin-wave peaks at smaller momenta. Analysis of this intriguing structure is in progress.

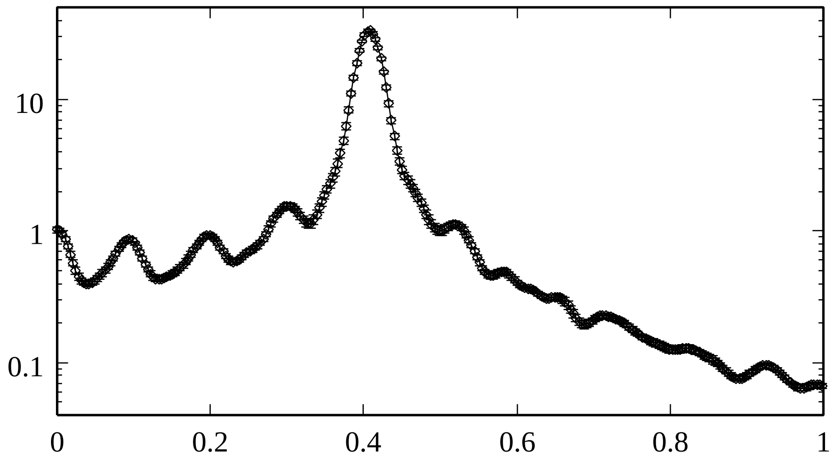

Figure 2: $S^{xx}(q,\omega)$ at $T = 0.600$, $L = 192$, $q = 8 \times \frac{2\pi}{L}$.

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