DYNAMIC SCALING IN THE TWO-DIMENSIONAL HEISENBERG ANTIFERROMAGNET

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INTRODUCTION

The two-dimensional Heisenberg antiferromagnet has generated considerable interest with respect to its applications for understanding copper-oxide-based high temperature superconductors.[1] The model is described by a Hamiltonian,

$$H = J \sum_{(n,m)} \vec{S}_n \cdot \vec{S}_m \tag{1}$$

where $J > 0$ and the sum is over nearest neighbor spin variables $\vec{S}_n$. While analytic calculations of either ground state or dynamic properties are very difficult for this and related nonlinear spin models, it is sometimes possible to extract important information from numerical calculations. Some success in obtaining ground state properties for the spin-1/2 model has resulted from quantum Monte Carlo calculations.[2] However, the principle interest here is in dynamics, for which quantum Monte Carlo calculations are emerging but not yet well-developed. Nevertheless, progress in obtaining quantities such as the dynamic structure function $S(q,\omega)$ is occuring.[3]

One important approach has been the dynamic scaling theory proposed by Chakravarty, Halperin and Nelson (CHN).[4] The CHN theory is based on a mapping (following that of Haldane[5]) of the quantum Heisenberg antiferromagnet onto an equivalent quantum O(3) nonlinear sigma model, whose properties are studied by including quantum fluctuations into a classical O(3) model. This equivalent classical model is a ferromagnetically coupled rotor model, whose Hamiltonian is

$$H = I \sum_n \frac{1}{2} \dot{\vec{\Omega}}^2_n - K \sum_{(n,m)} \vec{\Omega}_n \cdot \vec{\Omega}_m \tag{2}$$

where $\vec{\Omega}_n$ are the rotor variables with a kinetic energy in addition to the near-neighbor potential energy. The mapping is based on an assumption of low-energy perturbations about the classical antiferromagnetic ground state, and therefore is plausible at adequately low temperature, low frequency, and long wavelengths. The utility of the mapping is that it makes it possible to employ a numerical calculation of classical dynamics of the rotor model and then infer the corresponding quantum properties. This approach was followed by Tyc, Halperin and Chakravarty,[6] who made a simulation of the classical rotor model using Langevin dynamics, in an attempt to verify the dynamic scaling assumptions.

A related calculation[7] of dynamics is summarized here, but for the direct evaluation of spin dynamics of the two-dimensional classical Heisenberg antiferromagnet (Eq. 1). This excludes the quantum fluctuations but at the same time avoids the mapping to the rotor model; in the continuum limit the two models should be equivalent. Here we present a finite temperature simulation of the spin dynamics to produce $S(q,\omega)$, from which the wavevector and temperature dependence of the spinwave frequency ω_q and damping γ_q are estimated. These estimates are compared with the dynamic scaling theory.

DYNAMIC SCALING IN THE HEISENBERG ANTIFEROMAGNET

The principle quantity of interest is the dynamic structure function $S(q,\omega)$, defined in terms of the space- and time-displaced correlation function,

$$S(q,\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt \; e^{-i\omega t} \frac{1}{3} \langle \vec{S}_q(0) \cdot \vec{S}_{-q}(t) \rangle \tag{3}$$

where

$$\vec{S}_k(t) = \frac{1}{N} \sum_n e^{i\vec{k}\cdot\vec{r}_n} \vec{S}_n(t), \quad \vec{q} = (\pi,\pi) - \vec{k} . \tag{4}$$

The wavevector $\vec{q}$ is measured from the antiferromagnet Bragg point. In a scaling regime, (long wavelengths, low temperatures and frequencies) the scaling hypothesis assumes that there is an important physical length scale, which is the correlation length ξ, and a corresponding important time scale τ_s, or, correlation time, and these depend only on the temperature. Dynamical quantities measured at different temperatures will have their frequency and wavelength dependencies determined by the scaled wavevector, $Q \equiv q\xi$, and the scaled frequency, $\Omega \equiv \omega\tau_s$, rather than on q, ω and T separately. More specifically, the CHN scaling assumption for $S(q,\omega)$ is to write it in the form,

$$S(q,\omega) = \tau_s \, S(\vec{q}) \, \Phi(\vec{q}\xi, \omega\tau_s) \tag{5}$$

where $\Phi(Q,\Omega)$ is an undetermined scaling function. The amplitude is determined by the static structure function,

$$S(\vec{q}) = \frac{1}{3} \langle \vec{S}_q \cdot \vec{S}_{-q} \rangle \tag{6}$$

which itself displays scaling in the wavevector. Furthermore, the correlation length and time were shown to be related by[4]

$$\frac{\xi}{\tau_s} = \frac{c}{2\pi} \left(\frac{T}{2\pi J S^2} \right)^{1/2} \tag{7}$$

where c is the long-wavelength spinwave velocity.

The form of the scaling function is assumed here to be a product of Lorentzians,[8]

$$S(q,\omega) = \frac{A_q}{[(\omega+\omega_q)^2+\gamma_q^2]\,[(\omega-\omega_q)^2+\gamma_q^2]} \tag{8}$$

where the amplitude A_q, the spinwave frequency ω_q, and the damping γ_q are parameters to be fit in the numerical simulation. If scaling holds, then the spinwave frequency and damping must satisfy some scaling relationships,

$$\omega_q(T)=\omega_s(T)\ \Omega(q\xi), \qquad \gamma_q(T)=\omega_s(T)\ \Gamma(q\xi), \tag{9}$$

where $\Omega(Q)$ and $\Gamma(Q)$ are temperature-independent scaling functions, and $\omega_s \equiv 2\pi/\tau_s$.

NUMERICAL SIMULATION AND RESULTS

For finite temperature dynamics,[7] a classical Monte Carlo simulation was used to generate initial states for an energy-conserving spin dynamics integration of the equations of motion resulting from Hamiltonian (1). The MC calculation was also used to obtain the correlation length, ξ. Dynamic quantities were averaged over five initial states to produce an ensemble average. The calculations were performed using a 100 x 100 square lattice with periodic boundary conditions. A fourth order Runge-Kutta MD integration scheme was used, out to times $t \approx 250\ \hbar/JS$.

Some typical results for $S(q,\omega)$ are shown in Figure 1, together with the corresponding least square fits to Eq. (8). Similar fits to sums of Lorentzians were also made, but were not as good, with the fitted curves consistently being too low at low frequency and too high at high frequency. The damping, verses temperature, is shown in Fig. 2. At the lower temperatures, $T < 0.5$, the non-zero estimates of damping are due to the resolution of the simulation. The damping rate increases rapidly with q and T. The fitted spinwave frequency ω_q defined in Eq. (8) is shown verses wavevector in Fig. 3a. Softening with temperature is clear.

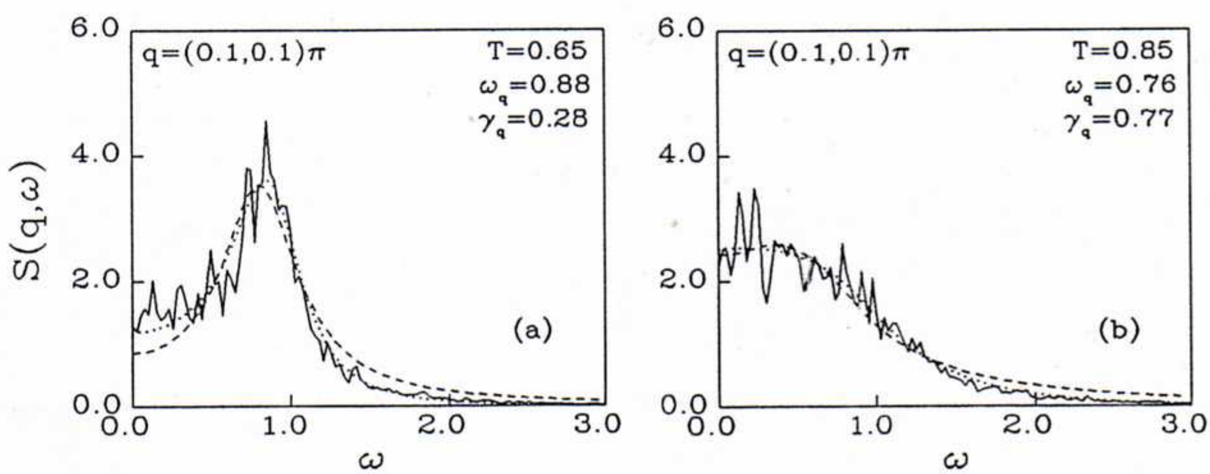

Fig. 1 Typical $S(q,\omega)$ data and curve fits for $q=(0.1,0.1)\pi/a$ at temperatures $T/JS^2=0.65$ and 0.85. The frequency is in units of $JS/\hbar$. The data were generated in the MCMD calculations described in the text. The dotted curve is a least-squares fit to a *product* of Lorentzians [Eq. 8], using spin-wave parameters shown. The dashed curve is a least-squares fit to a *sum* of Lorentzians for comparison (parameters not shown).

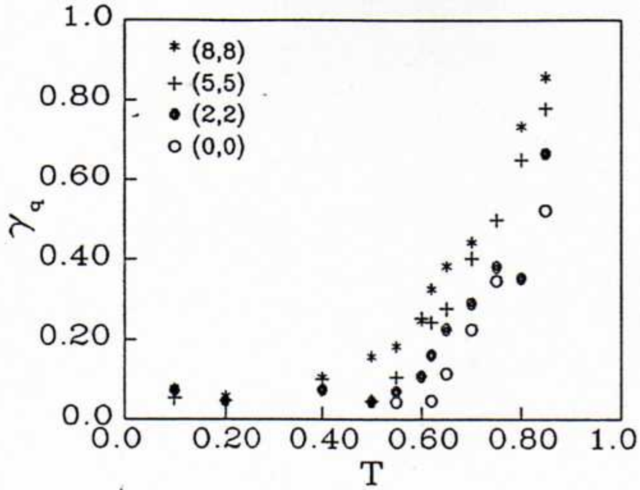

Fig. 2 The spin-wave linewidth γ_q vs. temperature for selected wave vectors q indicated in units of $\pi/50a$. The q=(0,0) data is used to give preliminary estimates of the scaling frequency ω_s.

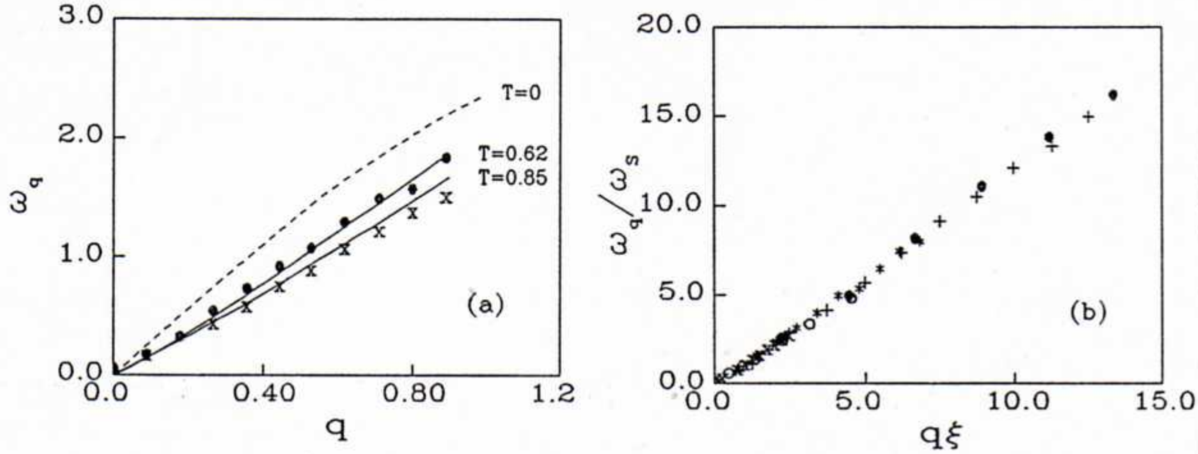

Fig. 3a Spin-wave frequencies ω_q vs. q, obtained from least-square fits as in Fig. 1. The MCMD data are compared with the zero-temperature dispersion, and the dispersion used in Ref. 6 [solid curves, with δ=2.5]. 3b) Scaled spin-wave frequencies ω_q/ω_s as a function of $q\xi$ using data derived at temperatures T/JS^2=0.62 (@), 0.65 (+), 0.70 (*), 0.75 (o), and 0.85 (x). Values of ω_s for each temperature (Table 1, Ref. 7) were first estimated from the q=0 linewidths in Fig. 2 and then corrected slightly such that the scaled frequencies from different temperatures fall on the same curve.

SCALING

The scaling frequency, ω_s, is proportional to the q=0 damping, $\gamma_{q=0}$, which can be read from Fig. 2 (open circles). Alternatively we can use the relationship to define the correlation time[7] τ_s,

$$\tau_s = \frac{\pi}{2} \frac{\int_{-\infty}^{\infty} dt\, S(q=0,t)}{S(q=0,t=0)} \tag{10}$$

For T > 0.6, ω_s increases approximately linearly with temperature. We have also found that the product, $\omega_s\xi$, first increases with T, but then decreases for T > 0.75, inconsistent with the CHN prediction, Eq.(7). This is probably because these temperatures are out of the range of validity of the CHN RG approach, which is an asymptotic theory ($T \rightarrow 0$).

The resulting scaled spinwave frequency, ω_q/ω_s, is shown in Fig. 3b, verses scaled wavevector, $Q = q\xi$, for a set of temperatures. The data at different T fall roughly along one curve, which defines the unknown scaling function, $\Omega(Q)$, and gives strong evidence for a scaling description. The damping rate verses Q determines $\Gamma(Q)$, but with less precision. In principle, even $\Phi(Q,\Omega)$ could be obtained by similar scaling methods but becomes technically difficult.

SUMMARY

The correlation length was estimated from the spatial decay of equal-time static correlations at long wavelengths ($q \rightarrow 0$ limit of Ornstein-Zernicke analysis). Correspondingly, the correlation time was estimated from the temporal decay of long wavelength ($q = 0$) correlations. The scaling theory is a long wavelength description but it should be kept in mind that damped propagating spinwaves make sense only when the wavelength is less than the correlation length ($q>\xi^{-1}$).

For the relatively high temperatures studied here, the dynamic structure function $S(q,\omega)$ is well-approximated by a product of symmetrically located Lorentzians. This implies that the spinwave correlations behave as a damped harmonic oscillator starting from rest with a finite initial displacement. The scaling function $\Phi(Q,\Omega)$ is similarly described by a product of Lorentzians. The spinwave frequency and damping were found to satisfy a scaling form. These results are consistent with earlier simulations of the classical rotor model.[6]

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