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Heisenberg Chains

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LOW TEMPERATURE SPIN WAVE DYNAMICS IN CLASSICAL HEISENBERG CHAINS*

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ABSTRACT

A detailed and quantitative study of the low-temperature spin-wave dynamics has been made for the classical Heisenberg-coupled chain using computer simulation. Results for the spin-wave damping rates and the renormalization of the spin-wave frequencies are presented and compared with existing predictions.

INTRODUCTION

The classical Heisenberg chain is one of the simplest magnetic models with an interesting dynamics - one which may be expected to approximate the behavior of real "one-dimensional" magnets[1]. This behavior includes a zero-temperature phase transition where dynamical scaling[2] may apply. Although the statics of this model are exactly soluble[3], the dynamics remain unclear despite numerous efforts[4-8] based primarily on moment extrapolations. The classical chain is ideal for study using computer simulation[9-12], since the Monte-Carlo procedure for generating an initial thermal equilibrium array can be done very efficiently[10,11]. Here we report a detailed and quantitative[13] simulation study of the spin-wave-like excitations at low temperatures, done for such systems of $N = 2400$ spins. Results for the spatially Fourier-transformed correlation function

$$C(q,t) = \sum_l e^{iqx} \langle S_0(0) \cdot S_l(t) \rangle \quad (1)$$

have been obtained both Ferro (F) and Antiferromagnetic (AF) coupling. The results presented here, which are confined to the regions of wave-vector and temperature where well defined spin-wave like excitations are observed, have been fitted to yield the spin wave frequencies ω and damping rates γ . The temperature dependence of γ and the q dependence of the spin wave renormalization are displayed graphically and compared with the predictions of Ref. 7 and with dynamic scaling.

NUMERICAL METHODS

Our techniques include a new method for solving the spin equations of motion for times up to ~ 200 units [14]. Also, in computing $C(q,t)$ the truncation of spatial correlations beyond $l_{\max} = 300$ has been handled quantitatively by introducing resolution correlations as follows: The spatial correlations $g_l(t) = \langle S_0(t_1) \cdot S_l(t_1+t) \rangle$ are first computed as in Ref. 11 except that an average over as many as 128 initial times t_1 could be taken using FFT methods[15]. This was repeated N_E times, each with an independent Monte Carlo initialization. (In practice N_E varied from 3 to 35.) To obtain results at wave-vector q_0 , we next computed the quantity

$$\tilde{C}(q_0, t) = \overline{g_0(t)} + 2 \sum_{l=1}^{l_{\max}} \overline{g_l(t)} e^{-\frac{1}{2}\sigma^2 l^2} \cos q_0 l, \quad (2)$$

the bars denoting an average over the repetition "ensemble". We chose σ to be small compared to the inverse correlation range, yet large enough so that $\exp(-\frac{1}{2}\sigma^2 l_{\max}^2) \ll 1$. Then, (for $N_E N \rightarrow \infty$) it may be shown that $\tilde{C}(q_0, t)$ is the convolution of the actual $C(q, t)$ with a resolution function $R \propto \exp[-(q-q_0)^2/2\sigma^2]$. The data analysis is then analogous to the method used in neutron scattering: $C(q, t)$ is parametrized in a physically reasonable form adequate to handle variations over the resolution width. We used the damped harmonic oscillator (DHO) form

$$C(q, t) = \chi e^{-\gamma t} [\cos(\omega_1 t) + (\gamma/\omega_1) \sin(\omega_1 t)] \quad (3)$$

where $\omega_1 = \sqrt{\omega^2 - \gamma^2}$. In fitting near each nominal wave-vector q_0 , we took $\chi(q)$, $\gamma(q)$, and $\omega(q)$ to be given by two or three term polynomials in $q-q_0$, the coefficients of the $q-q_0$ or $(q-q_0)^2$ terms being obtained from a preliminary fit to the data. The zero-order terms were left as adjustable parameters. A least-squares fit was then made of the resolution-convolution of (3) to the $\tilde{C}(q_0, t)$ data. Thus we found $\chi(q_0)$, $\gamma(q_0)$ and $\omega(q_0)$ for each q_0 . The expansion coefficients were then recalculated, and the procedure repeated if needed. To assess the statistical accuracy of the results, fits were also made to the $\tilde{C}(q_0, t)$ data for the individual "ensemble" members. The standard deviations in the resulting set of ω or γ values were calculated and divided by $\sqrt{N_E}$ to provide the standard deviation assigned to the ω or γ values found in the fit to the "ensemble average" data. The statistical accuracy of the computed correlation function $\tilde{C}(q_0, t)$ was similarly determined from the scatter about the "ensemble" mean.

RESULTS

In most cases the DHO form (3) gave an excellent fit. However, for $T=.3$ or $.2$ in the F case, with q between $\pi/2$ and π , the departures of the DHO fit from the data were beyond the statistical errors. The fitting was then done as follows: Eq. (3) was modified by replacing t by $t-\delta$ where δ is an adjustable parameter. The fit was then carried out deleting the data at short times. This gave good fits, with γ values reduced by up to 18%, and ω values increased by as much as 5% (or up to half the linewidth). Our intention in using this procedure was to determine the ω and γ values corresponding to the behavior in the "tail" of the curve, i.e. in the region in which the oscillation amplitude decreased from ~90% to ~10% of its initial value, generally speaking. The uncertainty in applying this procedure, folded with a two standard deviation statistical error, constitute the error bars shown in the figures.

For the F case the excitations were found to be well defined, (i.e. $\omega \gg \gamma$) when q was large compared with the inverse correlation range $\kappa = -\ln(-T + \coth T^{-1})/2T$. For the AF case this required that both q and $\pi-q$ be large compared with κ . These results are in harmony with dynamical scaling. For $q \ll \kappa$ the observed behavior was consistent with a diffusive exponential decay $C(q,t) \propto e^{-Dq^2 t}$. A quantitative study of the spin diffusion constant $D(T)$ is in progress and will be reported separately.

Our detailed results for the decay rates $\gamma(q,T)$ have been presented elsewhere[16]. For the AF case at each fixed T , γ depends only slightly on q , varying by less than $\pm 15\%$, and appearing to have a weak minimum just outside the critical region ($q \approx \pi$). This minimum moves further away from $q=\pi$ as the temperature is raised. To within the error limits, γ is found to be proportional to the temperature for each q studied. The observed weak q dependence within the spin wave regime is consistent with dynamical scaling given that $\gamma \propto T \approx \kappa$ at each such fixed q .

For the F case, γ peaks at or near $q=\pi/2$ at each temperature, the value there being proportional (and in fact equal) to the temperature to within the error limits. The q dependence for $q < \pi/2$ is approximately sinusoidal. To within the error limits we find

$$\begin{array}{l} q < \pi/2 \\ \text{F case} \end{array} : \quad \gamma(q,T) = (1 \pm 0.1) T \sin q. \quad (4)$$

This may be compared with the result of McLean and Blume[7] who find $\gamma = 2T \sin(q/2)$ or equivalently $\gamma = CTq$ for $\kappa \ll q < \pi/2$ with $C=1$. This latter form (with C unspecified) is just the result required by dynamical scaling with the additional assumption that $\gamma \propto \kappa$ for fix-

ed $q \gg \kappa$.

For $q=\pi$ in the F case the relaxation rate is definitely not proportional to the first power of the temperature. Instead our data give

$$\gamma(\pi, T) = (1.3 \pm 0.4) T^{1.5 \pm 0.2} \quad (5)$$

This is shown in Fig. 1 where we plot the relaxation rate as a function of the temperature for $q=\pi$ in the F case (lower curve), for $q=\pi/2$ in the F case (middle curve) and for $q=\pi/2$ in the AF case (upper curve). The

Fig. 1. Temperature dependence of the spin wave damping rate for $q=\pi$ and $q=\pi/2$ in the F case and $q=\pi/2$ in the AF case.

straight lines in the last two cases, drawn to have exactly unit slopes, are clearly close to optimal fits. By contrast, the slope for the F case with $q=\pi$ is decidedly greater than 1 as (5) shows. For $q=\pi/2$, the linewidth in the AF case is about 1.4 times that seen in the F case at the same temperature.

The spin wave frequencies $\omega(q, T)$ were generally found to agree within about one quarter of the linewidth with the results of Ref. 7, namely

$$\omega^2(q) = 4(1 - \cos q)^2(1 - T) + \frac{1}{2}T^2(1 - \cos q) \quad (6a)$$

for the F case and

$$\omega^2(q) = 4(1 - T)\sin^2 q + \frac{1}{2}T^2(1 - \cos q) \quad (6b)$$

for the AF case. Exceptions to this occurred for $T = .3$ or $.2$ in the F case, with q between $\pi/2$ and π . Here the fitted frequencies were systematically higher than those of Ref. 7 by up to $0.75 \gamma(q, T)$. (This discrepancy was greatly reduced when the simple ($\delta = 0$) DHO fit was used. However in this case, as already noted, the overall fit was poor.) At the lower temperatures Eqs. (6) provide a quite good account of the observed frequencies. To show this properly we plot the q dependence of the spin-wave renormalization

$$\Delta\omega(q, T) = \omega(q, 0) - \omega(q, T)$$

at $T = .1$ for the F and AF cases in Figs. 2 and 3 respectively. The solid curves drawn through the data points are guides to the eye, while the dashed curves represent $\Delta\omega$ as calculated from Eqs. (6). The vertical dashed line extensions of the error bars, terminating in the

Fig. 2. Spin wave frequency renormalization versus wave vector at $T = .1$ in the F case.

wedge marks, correspond to frequency ranges of plus or

6.

minus one linewidth γ . Thus while the experimental values do deviate systematically from the calculated values, the deviations are small relative to the linewidth. For the F case, $\Delta\omega$ is essentially always positive and given approximately by the simple formula $\Delta\omega = T(1 - \cos q) = \frac{1}{2}T\omega(q,0)$. Thus in the F case at low temperatures the fractional renormalization $\omega(q,T)/\omega(q,0)$ is approximately $1 - \frac{1}{2}T$. For the AF case, where $\omega(q,0) = 2 \sin q$, this simple expression for the fractional renormalization provides a fair description of $\Delta\omega$ for q values away from the critical region ($q \approx \pi$). However, as the critical region is approached, $\Delta\omega$ actually changes sign, as predicted by (6b). This is consistent with the fact that for AF coupling at $q = \pi$, ω vanishes

Fig. 3. Spin wave frequency renormalization versus wave vector at $T=.1$ in the AF case.

at $T=0$, while ω and γ appear experimentally to be comparable at finite low temperatures.

Following the completion of this work, we learned that Reiter and Sjölander have obtained a closed form for the spectral function which is asymptotically valid

in the zero temperature limit. The essential features of our numerical "experiments" appear in their theory. There are also significant detailed differences, as one would expect on the basis of the asymptotic character of their calculation. A full comparison of our results with theirs will be published elsewhere.

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FIG 1

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FIG. 3

November 1977

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