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Low-Temperature Spin-Wave Dynamics in Three-Component Classical Heisenberg Chains

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

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 solvable,[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] In this Letter we report the first 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,

$$C(q,t) = \sum_l e^{iql} \langle \vec{S}_0(0) \cdot \vec{S}_l(t) \rangle , \qquad (1)$$

are presented for both ferromagnetic (F) and antiferromagnetic (AF) coupling. These confirm some aspects of existing theories but are at vari-

ance with others.

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 $l_{\max} \simeq 300$ has been handled quantitatively by introducing resolution correlations as follows: The spatial correlations $g_l(t) = \langle \vec{S}_0(t_i) \cdot \vec{S}_l(t_i + t) \rangle$ are first computed as in Ref. 11 except that an average over as many as 128 initial times t_i could be taken using fast Fourier transform (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

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

the angular brackets 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 $N_E N \to \infty$) 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 $\omega_1 = (\omega^2 - \gamma^2)^{1/2}$. 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 zeroth-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 $C(q_0,t)$ 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.

In most cases the DHO form (3) gave an excellent fit. An example is given in Fig. 1, showing the fitted $\tilde{C}(q_0,t)$ data for $q = \pi/2$ at reduced temperature[14] $T = 0.1$ for the AF case. (The error

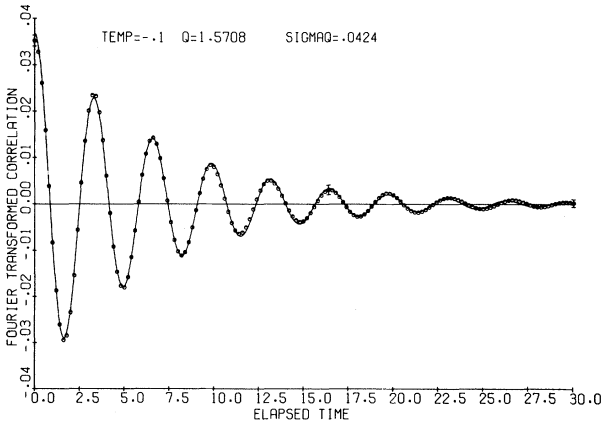

FIG. 1. Fitted observed correlation function $\tilde{C}(q_0,T)$ for $q_0 = \pi/2$, $T = 0.1$ with antiferromagnetic coupling. SIGMAQ is the σ of Eq. (2), and TEMP means k_B/J times the temperature. Error bars correspond to ± 2 standard deviations.

bars denote ± 2 standard deviations as determined "experimentally" from the scatter about the ensemble mean.) However, for $T = 0.3$ or 0.2 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. That this should happen was confirmed as follows: The DHO form cannot be correct since it has nonzero third and higher odd derivatives at $t = 0$. A reasonable *Ansatz* for the actual behavior is $C(q,t) = \chi e^{-L(t)} \cos\varphi(t)$, where L and φ are quadratic at short times, and become linear at long times, e.g., $\varphi(t) = \omega_1(t - t_s)$, where t_s is a small shift. Such a drift also appears for DHO, where $t_s = t_s{}^{\rm DHO} = \omega_1{}^{-1}\tan^{-1}(\gamma/\omega_1)$. To estimate the actual t_s, we employ a (tenth-order) moment expansion[6] to calculate the initial behavior of $C(q,t)$, finding the time $t = t_1$ of the first zero crossing. Assuming $t_s \ll t_1$, we have $t_s \approx t_1 - \pi/2\omega_1$, from which t_s could be estimated from our results for ω_1. This showed that $t_s \gg t_s{}^{\rm DHO}$ in just those cases where the fits to (3) were inadequate. The fitting was then done as follows: Equation (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%. Alternatively, we generated a model $C(q,t)$ curve by using the moment expansion for $t \leq t_1$, followed by a damped cosine for $t > t_1$, shifted and scaled so that the composite curve and its first derivative were continuous at t_1. This composite was then fitted with Eq. (3). The way in which the fitted γ and ω differed from the values used to generate the damped cosine part provided a correction for the

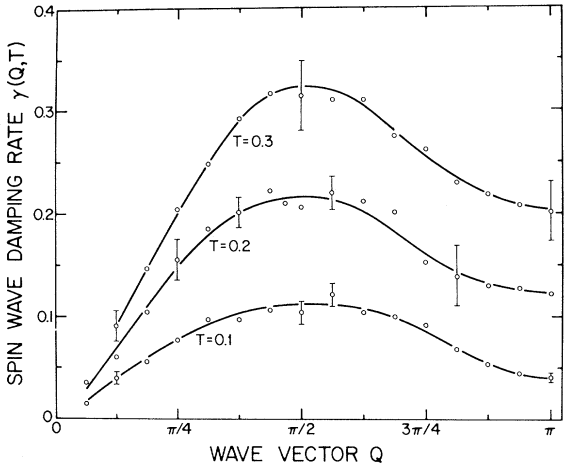

FIG. 2. Relaxation rates for ferromagnetic coupling at three temperatures. Drawn lines are guides to the eye. Error bars correspond to ±2 standard deviations.

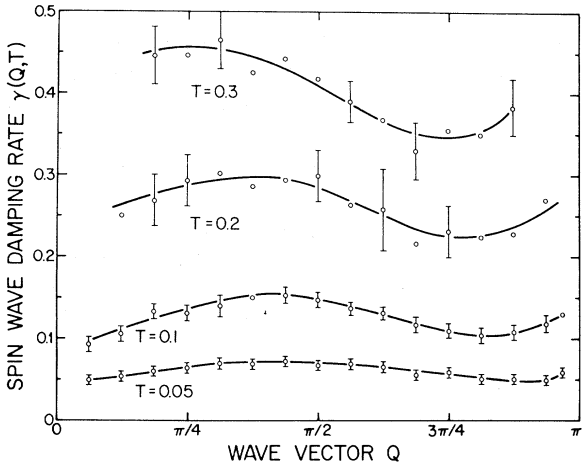

FIG. 3. Relaxation rates for antiferromagnetic coupling at four temperatures. Drawn lines are guides to the eye. Error bars correspond to ±2 standard deviations.

systematic errors due to the DHO form. These two techniques gave essentially equivalent results when they could both be reliably applied. Our intention in using them 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 uncertainties remaining after applying these procedures, folded with a 2-standard-deviation statistical error, constitute the error bars in Figs. 2 and 3.

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 $\kappa = \ln(-T + \coth T^{-1}) \cong T$. For the AF case, where this required that both q and $\pi - q$ be large compared with κ, ω and γ were found to be comparable at the critical wave vector $q = \pi$. These results are in harmony with dynamical scaling. For $q < \kappa$ 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.

In this Letter we present our results for the decay rates $\gamma(q, T)$ over the region where the excitations were well defined. For the F case, these are shown in Fig. 2. At each temperature γ peaks at or near $q = \pi/2$, the value there being proportional 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

$$\gamma(q, T) = (1.0 \pm 0.1)\kappa \sin q, \quad q < \pi/2 . \tag{4}$$

This may be compared with the result of McLean and Blume[7] who find $\gamma = 2\kappa \sin(q/2)$ or equivalently $\gamma = C\kappa q$ for $\kappa \ll q \ll \pi/2$ 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 fixed $q \gg \kappa$. The behavior for q comparable to the Brillouin-zone dimensions is, of course, not given by scaling. For $q = \pi$ our data give

$$\gamma(\pi, T) = (1.2 \pm 0.4)T^{1.45 \pm 0.2} . \tag{5}$$

The relaxation behavior for the AF case is shown in Fig. 3. Here the q dependence is much weaker: γ varies by less than ±15% at any given T, and appears to have a weak minimum just outside the critical region ($q \approx \pi$), this minimum moving 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 any q studied. The observed weak q dependence within the spin-wave region is again consistent with dynamical scaling and the additional constraint that $\gamma \propto \kappa$ at each fixed $q \gg \kappa$.

The spin-wave frequencies $\omega(q, T)$ were generally found to agree within $0.25\gamma(q, T)$ with the results of Ref. 7, namely $\omega^2(q, T) = 4(1 - \cos q)^2(1 - T) + \frac{1}{2}T^2(1 - \cos q)$ for the F case and $\omega^2(q, T) = 4(1 - T) \times \sin^2 q + \frac{1}{2}T^2(1 - \cos q)$ for the AF case. Exceptions to this occurred for $T = 0.3$ or 0.2 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 $0.75\gamma(q, T)$.

For none of the cases studied was there evi-

dence of a "central peak" of any appreciable weight in the corresponding spectral function. Observations at higher temperatures where such a peak may[5] occur will be carried out and reported separately.

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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Quantum Scattering Theory of Electron-Stimulated Desorption: Ion Angular Distributions

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This Letter presents a quantum scattering theory of electron stimulated desorption and applies it to recent observations of ion angular distributions. The Franck-Condon desorption cross section is calculated in a three-dimensional reflection approximation. It is shown that the adsorption models suggested by Madey, Czyzewski, and Yates, which attribute anisotropy in the angular distributions to initial-state effects, are consistent with the theory and the data.

Electron-stimulated desorption (ESD) has proven to be a useful tool in the study of adsorbed species on surfaces. The work of Redhead[1] and Menzel and Gomer[2] (RMG) served as an impetus for most of the modern work using this technique. Recently, Czyzewski, Madey, and Yates[3] reported the first observations of the angular distribution of ions in ESD. In their work on W(100)-O_2 some extremely interesting patterns were observed reflecting either the symmetry of the tungsten substrate, or the bonding oxygen adsorbate, or both. Shortly after this work, a more detailed report by Madey, Czyzewski, and Yates[4] (MCY) presented models to explain the previous data as well as more data corroborating their initial observations. In particular, they argue that the data for high-coverage β_1-oxygen, which exhibited fourfold-symmetric spot patterns, with and without central spots depending on the conditions, was due to tungsten-oxygen bonds normal and skew to the surface (i.e., WO and WO_2 configuration, respectively). These results are schematically rep-