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Exact Results for the Dynamics of the Classical Nearest-Neighbor Heisenberg Chain Near $T = 0$

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We present rigorous perturbation results for the dynamics of the classical nearest-neighbor Heisenberg chain, using the temperature as a small parameter. The lifetime and the frequency shift of the spin waves are determined. For the antiferromagnet we find that there is a region of wave vectors close to the zone boundary where the dynamical scaling fails and we argue that this is a general property of the Heisenberg chain close to $T = 0$.

We have calculated a rigorous perturbative expression for the spin-relaxation function of the classical, nearest-neighbor Heisenberg chain, using the temperature as the small parameter. The solution clarifies the physical origin of the damping at finite temperatures and the role that the constraint on the length of each spin, $\vec{S}_i \cdot \vec{S}_i = S^2$, plays in the dynamics. Rigorous results for the spin-wave damping and the frequency shift is given to lowest order in the temperautre. We find the dynamical scaling to hold near the zone center for the antiferromagnet and also for the ferromagnet within the region of validity of our calculations. At the zone edge we find for the antiferromagnet a region of wave vectors and temperatures where the dynamical scaling actually fails. This is characteristic of the Heisenberg chain and is not due to the perturbative treatment. The details of our derivation will be presented elsewhere and here we give only the basic steps and discuss the results.

As suggested in a comment by Mikeska,[1] we write the equation of motion for the Fourier components of the spin variables in the form

$$\frac{\partial^2 S_q^{\alpha}}{\partial t^2} = -\sum_{q_1,\ldots,q_3} \Gamma(q_1, q_2, q_3)\delta(q - q_1 - q_2 - q_3) S_{q_1}^{\alpha}\{\vec{S}_{q_2}\cdot\vec{S}_{q_3}\}. \tag{1}$$

This follows from the Hamiltonian

$$H = -J\sum_i \vec{S}_i \cdot \vec{S}_{i+1}, \tag{2}$$

and using the spin commutation rules, interpreted as Poisson brackets here. We have

$$\Gamma(q_1, q_2, q_3) = \tfrac{1}{2}[(J_{q_1+q_2} - J_{q_3})(J_{q_1} - J_{q_2}) + (J_{q_1+q_3} - J_{q_2})(J_{q_1} - J_{q_3})], \tag{3}$$

and $J_q = 2J\cos(qa)$, where J is the nearest-neighbor exchange constant and a is the nuclear lattice parameter. Using the exactly known static correlations, we find that

$$\langle(\delta\{\vec{S}_1\cdot\vec{S}_j\})^2\rangle = (n\kappa a)^2 \text{ for } \kappa|\vec{r}_i - \vec{r}_j| \ll 1, \tag{4}$$

where $\delta\{\vec{S}_i\cdot\vec{S}_j\} = \vec{S}_i\cdot\vec{S}_j - \langle\vec{S}_i\cdot\vec{S}_j\rangle$ represents the fluctuation from the equilibrium average value and $na = |\vec{r}_i - \vec{r}_j|$ is the distance between the two spins. The coherence length $\kappa^{-1} = JS^2a/KT$, and S is the length of each spin. For $n=0$, Eq. (4) expresses the constraint $\vec{S}_i\cdot\vec{S}_i = S^2$ and for $n>0$ it shows that the fluctuation $\delta\{\vec{S}_i\cdot\vec{S}_j\}$ is small when the separation of the spins is much less than the coherence length. Since the coefficient Γ restricts the distance between sites appearing in (1) to at most two lattice spacings, the fluctuations will, on the average, be small for low temperatures. Neglecting these one obtains sharp spin waves with a frequency

$$\omega_{q,T}^2 = \sum_{q'}\Gamma(q, q', -q')\langle\vec{S}_{q'}\cdot\vec{S}_{-q'}\rangle, \tag{5}$$

which for $T=0$ gives the correct spin-wave frequencies, $\omega_{q,0} = 4JS\sin^2(qa/2)$ (ferromagnet) and $\omega_{q,0} = 2|J|S\sin(qa)$ (antiferromagnet). The damping at finite temperatures is due to fluctuations in $S_{q_1}{}^{\alpha}\delta\{\vec{S}_{q_2}\cdot\vec{S}_{q_3}\}$ and we find that the fluctuations in $\delta\{\vec{S}_{q_2}\cdot\vec{S}_{q_3}\}$ are the important ones at low temperatures. In the dynamical spherical model, where $\vec{S}_i\cdot\vec{S}_i$ can fluctuate subject only to the constraint $N^{-1}\sum\vec{S}_i\cdot\vec{S}_i = S^2$, there are no well-defined spin waves for $T\to 0$,[2-4] and we therefore conclude that the constraint is playing a crucial role here.

To obtain the damping systematically we apply the Zwanzig-Mori projection-operator technique and write the Laplace transform of the spin-relaxation function in the form

$$\Sigma(q, z) = \int_0^\infty dt\, e^{izt}\langle\vec{S}_q(t)\cdot\vec{S}_{-q}(0)\rangle = i\langle\vec{S}_q\cdot\vec{S}_{-q}\rangle\{z - \omega_q^2[z + \gamma_q(z)]^{-1}\}^{-1}, \tag{6}$$

where ω_q^2 is the second moment of $\Sigma(q, z)$. The function $\gamma_q(z)$ can be interpreted as the frequency- and wave-vector-dependent "decay rate" for the spin current and can be expanded in a power series in the temperature if we neglect terms of order $\exp(-2JS^2/KT)$, i.e.,

$$\gamma_q(z) = JS[\kappa a\gamma_{q,1}(z) + (\kappa a)^2\gamma_{q,2}(z) + \ldots]. \tag{7}$$

It is possible to calculate $\gamma_{q,1}(z)$ exactly. $\gamma_q(z)$ is determined by the correlation function $\langle S_{q_1}{}^{\alpha}(t) \times\delta\{\vec{S}_{q_2}(t)\cdot\vec{S}_{q_3}(t)\}S_{q_1'}{}^{\alpha}\delta\{\vec{S}_{q_2'}\cdot\vec{S}_{q_3'}\}\rangle$. T lowest order in T, the time dependence of $S_q{}^{\alpha}$, plays no role and one may evaluate the time dependence of $\delta\{\vec{S}_{q_2}(t)\cdot\vec{S}_{q_3}(t)\}$ from an equation of motion valid at $T=0$. $\gamma_{q,1}(z)$, for both ferromagnet and antiferromagnet, can be represented as $(z^2 - \omega_{q,0}{}^2)z^{-1} \times\gamma_{q,1}'(z)$, where for the ferromagnet

$$\gamma_{q,1}'(z) = \tfrac{1}{2}(J/KT)^2\omega_{q,0}\sum_{q',q''}\sin^2(q'a)\sin^2(q''a) \times[z^2 - (\omega_{q/2-q',0} - \omega_{q/2+q',0})^2]^{-1}\langle\delta\{\vec{S}_{q/2+q'}\cdot\vec{S}_{q/2-q'}\}\delta\{\vec{S}_{-(q/2+q'')}\cdot\vec{S}_{-(q/2-q'')}\}\rangle. \tag{8}$$

A similar expression holds for the antiferromagnet. As is evident from (8), the damping mechanism is the resonant absorption by pairs of spin waves. Equation (8) and its analog for the antiferromagnet reduce the problem to the evaluation of certain integrals containing the static correlation functions. These are readily computed[5] and the integrations performed by contour integrations. The spectral function is now obtained from (6) with the replacement of $\gamma_q(z)$ by $(KT/S)\gamma_{q,1}(z)$ and use of

$$\omega_q^2 = (2JS)^2\kappa a[1 - \cos(qa)][1 + y^2 - 2y\cos(qa)]y(1-y^2)^{-1}, \tag{9}$$

where $y = \pm(1-\kappa a)$, when exponentially small terms are neglected. The plus and minus signs refer to the ferromagnetic and antiferromagnetic case, respectively. The spectral function obtained in this way will have all moments correct to first order in κa, i.e., if $\omega_q^{2n} = (\omega_{q,0}{}^2)^n + \kappa a A_q{}^n + O((\kappa a)^2)$ then $A_q{}^n$ will be exact. In particular, the results agree with those of Tomita and Mashiyama for the moments up to the sixth when these are expanded to first order in κa.

For the ferromagnet, terms in (7) that are of higher order in κ, but lower order in q, dominate $\gamma_q(z)$ for $q<\kappa$, and our results are therefore restricted to $q>\kappa$. For the antiferromagnet the lowest-order term in κ is also lowest order in q and $q^* = \pi - q$ and there is no restriction. The final results are presented below.

(a) For the ferromagnet ($J>0$) and $q>\kappa$,

$$\gamma_{q,1}(\omega) = -2\sin(qa/2)[\zeta - (\zeta^2-1)^{1/2} + (\zeta^2-1)^{-1/2}\cos^2(qa/2)], \tag{10}$$

where $\zeta = \omega[4JS\sin(qa/2)]^{-1}$. For $\zeta<1$, $(\zeta^2-1)^{-1/2}$ and $(\zeta^2-1)^{-1/2}$ go over to $i(1-\zeta^2)^{1/2}$ and $-(1-\zeta^2)^{-1/2}$, respectively. We obtain for $T\to 0$ sharp, essentially Lorentzian spectral lines around

$$\omega = 4JS\sin^2(qa/2)[1 - KT(2JS^2)^{-1}] \tag{11}$$

for all q values. However, the tail of the spectral function always drops to zero when $\omega > 4|J|S\sin(qa/2)$, implying that all higher-order moments do exist. The half-width of the spin resonance is, except near $q=\pi/a$,

$$\Delta_q = KT(JS^2)^{-1}JS\sin(qa). \tag{12}$$

Close to $q=\pi/a$, the linewidth is proportional to $T^{3/2}$. These results are quite different from what has been found before in approximate treatments.[4-8] For small wave vectors we can introduce the scaled variables $\tilde{q}=q/\kappa$ and $\tilde{\omega}=\omega/|J|Sa^2\kappa^2$ and write

$$\mathrm{Re}\Sigma(q,\omega)/\langle\vec{S}_q\cdot\vec{S}_{-q}\rangle = (JS\kappa^2a^2)^{-1}2\tilde{q}^5(1+\tilde{q}^{-2})[\tilde{\omega}^2 - \tilde{q}^2(1+\tilde{q}^2) + (2\tilde{\omega}\tilde{q})^2]^{-1}. \tag{13}$$

The solution satisfies the dynamical-scaling hypothesis with a characteristic exponent $z=2$. Note that the scaling property is violated when ζ becomes of order unity, which implies $\omega\sim 2\tilde{q}/\kappa a$ or alternatively $\omega\sim 2JSqa$. Thus, the scaling is violated long before values of ω of order JS are reached.

(b) For the antiferromagnet $(J<0)$,

$$\gamma_{q,1}(\omega) = -2\sin(qa/2)[\zeta_1 - (\zeta_1^2-1)^{1/2}] - 2\cos^3(qa/2)[\zeta_2^2-1]^{-1/2}, \tag{14}$$

where $\zeta_1=\omega/4|J|S\sin(qa/2)$ and $\zeta_2=\omega/4|J|S\cos(qa/2)$. As before we should replace $(\zeta^2-1)^{1/2}$ and $(\zeta^2-1)^{-1/2}$ by $i(1-\zeta^2)^{1/2}$ and $-i(1-\zeta^2)^{-1/2}$, respectively, for $\zeta<1$. We have to consider separately $q\approx 0$ and π/a; elsewhere we have an essentially Lorentzian spectral-line shape around the resonance frequency

$$\omega = 2|J|S\sin(qa)[1 - KT(2JS^2)^{-1}], \tag{15}$$

with the width,

$$\Delta_q = KT(JS^2)^{-1}JS, \tag{16}$$

being independent of q. Again, for small values of qa we may introduce scaled variables $\tilde{q}=q/\kappa$, $\tilde{q}^*=q^*/\kappa$, and $\tilde{\omega}=\omega/2|J|Sa\kappa$. We have then

$$\mathrm{Re}\Sigma(q,\omega)/\langle\vec{S}_q\cdot\vec{S}_{-q}\rangle = (2|J|S\kappa a)^{-1}\tilde{q}^2[\tilde{\omega}^2-\tilde{q}^2)^2+\tilde{\omega}^2]^{-1}, \tag{17}$$

except far out in the wings. This gives for $\tilde{q}^2\gg\frac{1}{2}$ sharp resonances at $\tilde{\omega}=\pm(\tilde{q}^2-\frac{1}{2})^{1/2}$. For $\tilde{q}^2\ll\frac{1}{2}$ we obtain essentially a Lorentzian line shape around $\omega=0$ and for the corresponding spin-diffusion constant we have $D=2|J|Sa/\kappa$. The situation is more complicated close to $qa=\pi$. There the term $(\zeta_2^2-1)^{-1/2}=(\tilde{\omega}^2/\tilde{q}^{*2}-1)^{-1/2}$ diverges and the last term in (14) can dominate. Near $q^*=0$ we have

$$\Sigma(q,\omega)/\langle\vec{S}_q\cdot\vec{S}_{-q}\rangle = i(2|J|S\kappa a)^{-1}\{\tilde{\omega} - (1+\tilde{q}^{*2})[\tilde{\omega} + i(1+\tfrac{1}{8}\kappa^3a^3\tilde{q}^{*4}(\tilde{q}^{*2}-\tilde{\omega}^2)^{-1/2})]^{-1}\}^{-1}. \tag{18}$$

Except at $q^\alpha=0$, the solution does not satisfy the dynamical-scaling hypothesis, because of the singular term in (18).[9] This is not an artifact of the perturbation treatment and would not be eliminated by higher-order terms, as will be argued below. If we denote by $\kappa a\tilde{\gamma}_q(\omega)$ the difference $[\gamma_q(\omega) - \kappa a\gamma_{q,1}(\omega)]$, then $\tilde{\gamma}_q(\omega)$ is a function whose moments are all of order κa or higher. Both γ_q and $\gamma_{q,1}$ obey the Kramers-Kronig relations, and hence so does $\tilde{\gamma}$. From the representation of the moments of $\tilde{\gamma}$ as integrals over the imaginary part, $\gamma_q''(\omega)$, it follows that $\gamma_q''(\omega)$ can be of order unity only over an interval that vanishes as κa, and must be of order κa in any interval of fixed length. But the singular term in (18) is of order unity over an interval $\Delta\omega\simeq|J|S(q^*a)^7(128)$ which is independent of κa. Hence for sufficiently small κa, the higher-order terms cannot cancel the singularity. There is a region in the q^*-κ plane, determined by $1\gg q^*a\gg(\kappa a)^{1/7}$, where the dynamical scaling certainly fails. Ultimately, the breakdown of the scaling is due to the detailed effect of the constraint on $\vec{S}_i\cdot\vec{S}_i$, since the one-dimensional dynamical spherical model satisfies the scaling hypothesis.

The existance of singularities in the higher-order terms of $\gamma_q(\omega)$ at $\omega=0$ could invalidate the results for the width and the line shape at $q<\kappa$ and $q^*<\kappa$. We have not been able to rule this out on mathematical or physical grounds. However, if we assume that dynamical scaling holds near the

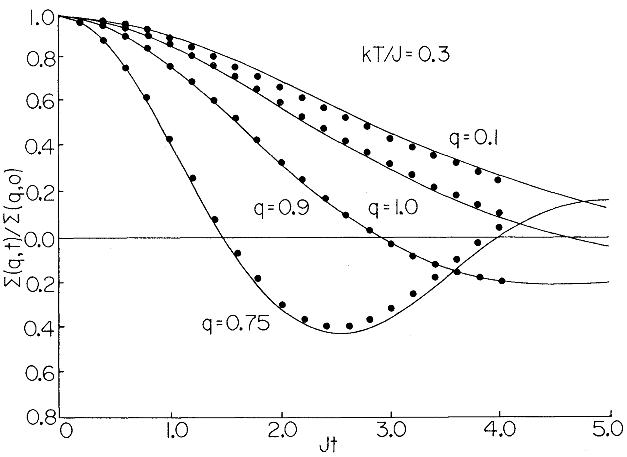

FIG. 1. Comparison of numerical calculations of Windsor and Locke-Wheaton (Ref. 10) (dots) with theoretical result (solid line). The discrepancies are within the statistical error of the numerical calculations. q is in units of π/a. Temperature and time are in such units that $S = 1$.

zone center and that the spectrum for $q \ll \kappa$ is rigorously diffusive, then the diffusion constant we have obtained can be proven to be exact. In Fig. 1 we show the comparison with the computer simulations of Windsor and Locke-Wheaton (WLW)[10] for the antiferromagnet at $KT/JS^2 = 0.3$. The differences that exist are within the statistical uncertainty of their numerical calculations. This remains true also for the calculations of Blume, Vineyard, and Watson (BVW)[11] at $q = \pi/a$, which are available up to $JSt = 7$. The solution for the ferromagnet and the antiferromagnet at $q = \pi/2a$ are identical, and the BVW data show clearly this equivalence. The comparison with WLW at lower temperatures give the same good agreement. Any signularities in the higher-order terms must have very small strength. If $|\gamma_q(\omega) - JS\kappa a \gamma_{q,1}(\omega)|/(\kappa a)^2$ is bounded, independent of κa, then the spectral function is asymptotically exact in the limit $T \to 0$.

For not-too-low temperatures, we find that the line shapes are far from Lorentzian, falling off more rapidly on the high-frequency side, and this affects significantly the evaluation of the width at half-maximum. Detalied comparisons with experimental and molecular-dynamics data will be presented elsewhere.[12]

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[12]After submission of this work we learned that P. Heller and M. Blume [Phys. Rev. Lett. 39, 962 (1977)] have obtained the correct wave-vector and frequency dependence of the linewidths, including the $T^{3/2}$ dependence in the ferromagnet at the zone corner; their computer simulations were carried out to much longer times than those reported here.