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# Zero-Temperature Dynamics of the $S=\frac{1}{2}$ Linear Heisenberg Antiferromagnet

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We present an analytical expression for the dynamical spin-correlation function of the $S=\frac{1}{2}$ linear Heisenberg antiferromagnet based on the fact that the spectrum is dominated by a double continuum of spin-wave excitations. Our expression is not exact, but exact sum rules show that the degree of approximation is small. We predict that in a uniform magnetic field the spectral weight function will display a double-peaked structure. Such a feature is observed in recent neutron-scattering experiments.

Spin dynamics is a subject of considerable current interest and activity, whose development is hampered considerably by lack of exact results, particularly for Heisenberg systems. Even in one dimension (1D), calculations have relied heavily on the classical (spin $S=\infty$) Heisenberg chain, despite abundant evidence that quantum effects are extremely important at low temperatures ($T\rightarrow 0$). The problem is that for the quantum, $S=\frac{1}{2}$, Heisenberg chain, exact results are limited, even for the simpler problem of the static thermodynamic quantities.[1] Fortunately, extensive numerical calculations[2] have provided considerable information and understanding. Knowledge of the antiferromagnetic (AFM) spectral excitations is limited to the des Cloizeaux–Pearson (dCP) dispersion-curve calculations[3] recently extended by Ishimura and Shiba[4] to the case of nonzero applied magnetic field $H$. Exact results for the spin correlations, and hence the spin dynamics, are totally lacking. Exact (or reliable numerical) calculations would therefore be most timely, and valuable in several ways. Because of the great void indicated above,[5] such results would (a) substantially advance our understanding of the AFM Heisenberg linear chain, (b) provide qualitative and quantitative estimates of important quantum effects, for example, asymmetrical line shapes observed in neutron scattering experiments on the linear AFM, $CuCl_2 \cdot 2N(C_5D_5)$ (dichloro *bis*-pyridine copper II, abbreviated as CPC),[6,7] and (c) offer testing possibilities for 3D approximate theories. Furthermore, calculations in nonzero $H$ are needed (d) for spin Peierls systems in a field, and (e) to explain features of more recent neutron-scattering experiments on CPC for $H>0$, particularly the appearance of a double peak in the spectral weight distribution at 70 kOe.[6]

Here we synthesize information obtained from (a) exact calculations on finite chains of two through ten spins; (b) from selection rules which show exactly which classes of states have nonzero matrix elements with the ground state (and hence contribute to the spin dynamics) for both $H=0$ and $H>0$; (c) from sum rules; and (d) from both exact and approximate dispersion curves. We feature an analytic expression for the dynamical correlation function in $(q, \omega)$ space derived using the above information. Although not rigorous, the expression yields good agreement with the few known exact results for the $S=\frac{1}{2}$ chain, and, most important, allows for the first quantitative interpretation of the results of neutron-scattering experiments.

It was pointed out recently[8-10] that the dCP excitations were not the dominant feature of the $H=0$ spectrum, but merely formed the lower boundary of a triplet (total spin $S=1$) continuum. This spin-wave continuum is actually a double (i.e., two-parameter) continuum in $(q, \omega)$ space, and is hereafter denoted SWDC. Exact calculations show that there is an upper boundary to the SWDC given by $E_2(q)=\pi J|\sin(\frac{1}{2}q)|$,[8,10] whereas the dCP expression is $E_1(q)=(\frac{1}{2}\pi J)|\sin q|$, if we consider the isotropic, $S=\frac{1}{2}$ chain with Hamiltonian $H=J\sum_i \vec{S}_i \cdot \vec{S}_{i+1}$. It should be noted that the Anderson spin-wave result is actually the dispersion curve for the classical $(S=\infty)$ chain, $E^{\mathrm{cl}}(q)=J|\sin q|$. The pattern of low-lying states of the AFM chain is quite complicated (see Fig. 1 of Ref. 8), involving singlet $(S=0)$ and quintet $(S=2)$ as well as triplet states. Fortunately, we can prove selection rules which show that the only states having nonzero matrix elements with the (singlet) ground state are triplets.

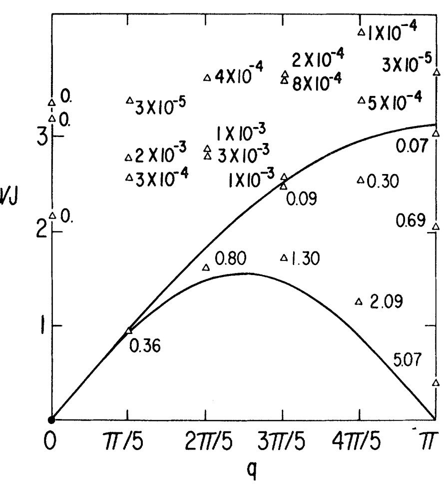


FIG. 1. $G_{zz}(q, \omega)$ for a cyclic chain of $N=10$ spins. For each $q$, $G_{zz}(q,\omega)$ is a sum of $\delta$ functions. The open triangles denote energy and wave number of the triplet excitations, and the numbers represent the corresponding spectral weight. At higher energies there are more triplets, not shown with very little spectral weight. No other excitations have nonzero matrix elements. The solid circle indicates the singlet ground state. The two solid lines represent $E_1(q)$ and $E_2(q)$ which form the lower and upper boundary of the SWDC in the thermodynamic limit.

Figure 1 shows the spectral weights for the triplet states for a ten-spin ring. We may note the following: (a) Almost all the spectral weight is concentrated within the boundaries of the SWDC; (b) the matrix elements increase in magnitude as the energy decreases to the lower (dCP) boundary, $E_1(q)$; and (c) there is some very small but finite weight well above $E_2(q)$. Exact sum-rule results of Hohenberg and Brinkman[9] and finite-chain calculations[11] indicate that this weight should persist in the thermodynamic limit.

The dynamical spin-correlation function in $(q, \omega)$ space, $G_{zz}(q,\omega)$ is the Fourier transform of $\langle S_l^z(t) S_{l'}^z(0)\rangle$, and is proportional to the inelastic-neutron-scattering cross section. We denote the dominant part of $G_{zz}(q,\omega)$, which comes from the SWDC, as $G_{zz}^{\mathrm{SWDC}}(q,\omega)$. We postulate the following analytical form for $G_{zz}^{\mathrm{SWDC}}(q,\omega)$, and later test it in the light of exact sum rules and experimental results:

$$G_{zz}^{\mathrm{SWDC}}(q,\omega) \propto [\omega^2 - E_1^2(q)]^{-\varphi}\theta(\omega - E_1(q))\theta(E_2(q)-\omega), \quad (1)$$

where $\theta$ is the step function.

This function diverges at the lower threshold energy, $E_1(q)$, and has a smoothly decreasing tail up to $E_2(q)$, the upper, cutoff energy. This form is in agreement with a semiclassical calculation of Mikeska[12] for $q \sim \pi$ and $T=0$, and with correlation functions derived from a continuum lattice (Luttinger) model of Luther and Peschel[13]

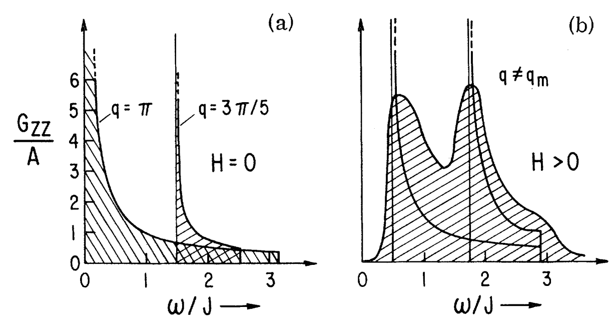


FIG. 2. (a) $G_{zz}^{\mathrm{SWDC}}(q,\omega)$ in zero field for two different $q$ values: $q=3\pi/5$ and $q=\pi$. (b) Sketch of $G_{zz}(q,\omega)$ for $H>0$, for a *single* $q$, $q\neq q_m$. Two divergences result at $T=0$, corresponding to the two partly overlapping continua. The effect of $T>0$ is shown as the shaded sketch, illustrating the double peak.

for $q \sim 0$ and $q \sim \pi$. The introduction of an upper cutoff at $E_2(q)$ is an important new feature of our calculations. $E_2(q)$ and $E_1(q)$ are the upper and lower boundaries of the SWDC, and the Luther-Peschel calculation indicates that $\varphi = \frac{1}{2}$. Hence, explicitly,

$$G_{zz}^{\mathrm{SWDC}}(q,\omega) = A[\omega^2 - (\tfrac{1}{2}\pi J)^2 \sin^2 q]^{-1/2}\theta(\omega - \tfrac{1}{2}\pi J \sin q)\theta(\pi J \sin(\tfrac{1}{2}q) - \omega). \qquad (2)$$

$G_{zz}^{\mathrm{SWDC}}(q,\omega)$ is sketched in Fig. 2(a) for two $q$ values. The jump at the upper cutoff depends on the constant $A$, which will be approximately determined from sum rules.

Three simple sum rules link $G_{zz}(q,\omega)$ to various static quantities. The first relates $G_{zz}(q,\omega)$ to the static susceptibility

$$\chi_{zz}(q) \equiv (1/2\pi)\int_0^\infty d\omega\, \omega^{-1} G_{zz}(q,\omega). \qquad (3)$$

On substitution of (2), we obtain $\chi_{zz}^{\mathrm{SWDC}}(q) = (A/2\pi^2 J)q/\sin q$. For comparison, the classical result is $\chi_{zz}^{\mathrm{cl}}(q) \equiv [3J(1+\cos q)]^{-1}$, which has a different divergence at $q = \pi$.

A second sum rule relates $G_{zz}$ to the ground-state energy, which is known exactly:

$$K_{zz}(q) \equiv (1/2\pi)\int_0^\infty d\omega\, \omega G_{zz}(q,\omega)$$

$$= -(4E_0/3N)(1-\cos q), \qquad (4)$$

where $E_0 = -JN(\ln 2 - \frac{1}{4})$. For our $G_{zz}^{\mathrm{SWDC}}(q,\omega)$, we obtain $K_{zz}^{\mathrm{SWDC}}(q) = (AJ/4)(1-\cos q)$, which reproduces the correct $q$ dependence. This result *validates* the introduction of $E_2(q)$ as an upper cutoff for $G_{zz}^{\mathrm{SWDC}}$.

We may now use (3) and (4) to determine the constant $A$. The susceptibility is known exactly at $T = 0$ and $q = 0$ to be $\chi_{zz}(0) = (\pi^2 J)^{-1}$,[14] which implies that $A = 2$. For agreement with (4), however, we must require that $A = \frac{16}{3}(\ln 2 - \frac{1}{4}) \simeq 2.3635\ldots$. The discrepancy is attributed to the approximate nature of our $G_{zz}^{\mathrm{SWDC}}$, which neglects the effect of higher triplet excitations[9,11] included in the complete $G_{zz}(q,\omega)$.

A third frequency moment gives the static correlation function of integrated intensity,

$$C_{zz}(q) \equiv (1/2\pi)\int_0^\infty d\omega\, G_{zz}(q,\omega), \qquad (5)$$

from which we obtain $C_{zz}^{\mathrm{SWDC}}(q) = (A/2\pi)\ln[(1+|\sin(\frac{1}{2}q)|)/\cos\frac{1}{2}q]$. This contrasts with the classical spin-wave result based on the fully aligned Néel state, $C_{zz}^{\mathrm{cl}}(q) = |\tan(\frac{1}{2}q)|$. $C_{zz}(q)$ itself must fulfill a sum rule

$$(1/2\pi)\int_{-\pi}^{\pi} dq\, C_{zz}(q) = \langle (S_l^z)^2\rangle = \tfrac{1}{4}, \qquad (6)$$

which forbids a power-law divergence of $C_{zz}(q)$ at the zone boundary ($q = \pi$), such as occurs in the classical case, but allows a weaker logarithmic divergence. This is consistent with a conjecture from finite-chain calculations that $C_{zz}(\pi)$ $\propto \ln N$.[2,15] A third independent determination of $A$ may be made from (6). A value of 1.35 is obtained, which, in comparison with values of 2 and 2.3635... gives a feeling for the accuracy and consistency of our analytic expression. We might suggest a "best" value for $A$ of about 2. Present experimental results are not sensitive to the value for $A$.

The experimental predictions associated with our expression for $G_{zz}(q,\omega)$ are that neutron-scattering line shapes at low $T$ should appear fairly symmetric at small $q$, but develop a marked asymmetry as $q$ approaches $\pi$. This phenomenon is indeed observed in recent experimental work by Heilmann *et al.*[6] It can be seen in Ref. 7 (Fig. 4) that the experimental data for CPC lie consistently below $C_{zz}^{\mathrm{cl}}(q)$. The data, however, are quantitatively consistent with our $C_{zz}^{\mathrm{SWDC}}(q)$, which diverges more weakly [as $|\ln(\pi - q)|$ rather than $(\pi - q)^{-1}$] as $q \to \pi$.

Having established that the spin dynamics in $H = 0$ is dominated by a triplet SWDC, we now proceed to examine the more complicated situation for $H > 0$, not previously theoretically investigated. For the case of a uniform magnetic field parallel to the $z$ axis, there exist two partially overlapping double continua, instead of one, as shown in Fig. 3. This result follows from (a) finite-chain calculations, (b) exact selection rules which show that *two* distinct classes of states exist with nonvanishing matrix elements when $H < 0$, and (c) comparison with the $XY$ model for which exact results are available. Again, the spectral weight of $G_{zz}(q,\omega)$ increases towards the lower edge of each continuum, as sketched in Fig. 2(b). Therefore we predict that low-temperature neutron scattering will reveal double-peak structure, except at $q = \pi$, where the boundaries meet. This two-peak structure is indeed observed in experiments on CPC in a field of 70 kOe.[6]

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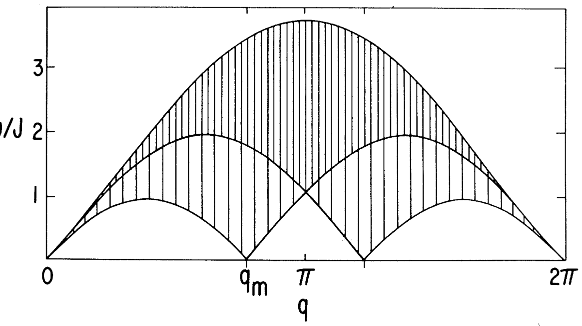


FIG. 3. The two continua of excitations dominating $G_{zz}(q,\omega)$ at $T=0$ and $H=\frac{1}{2}H_{\text{crit}}$. They have a common upper boundary. In each continuum the spectral weight increases strongly towards the corresponding lower boundary. The lowest boundary corresponds approximately to the Ishimura-Shiba spin-wave frequency (see Ref. 4). The special wave number $q_m$ depends only on the magnetization. It is equal to $\pi$ at $H=0$ and decreases as $H$ increases, reaching zero at the critical field $H_{\text{crit}}$.

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# Duality, Solitons, and Dilute-Gas Approximation in the One-Dimensional $X$-$Y$ Model with Symmetry-Breaking Fields

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The continuous–transfer-matrix technique, together with the dilute-gas approximation, is used to study the thermodynamics and static properties of the linear-chain planar model. Explicit analytic expressions for the free-energy and spin-spin correlation functions, as a function of temperature, symmetry-breaking fields, and density of solitons, are given. The correlation length is predicted to increase exponentially as the temperature goes to zero. This result should be seen in elastic neutron scattering experiments on $CsNiF_3$.

In a recent paper Kjems and Steiner[1] (KS) argued that the central peak found in their neutron scattering experiment on $CsNiF_3$ in the presence of an external magnetic field is clear evidence for the existence of soliton excitations. KS founded their assertions on Mikeska's[2] results for the spin-spin dynamic correlation function (SSCF) for the ferromagnetic planar model which has been shown[3] to represent $CsNiF_3$ at low temperatures. Mikeska considered the soliton contribution to SSCF but did not study the relevance of the other excitations in the problem, namely, magnons, breathers, and the coupling between them. Moreover, it is not obvious that the SSCF decouples to give an independent soliton branch in the dynamic structure factor which was the basis for Mikeska's argument.

In this paper we present a systematic analysis of the equilibrium properties of the planar model with and without symmetry-breaking fields. Our analysis takes into account, *from the start*, the presence of the solitons in the model. From our results we can actually see how the decoupling of the dynamic SSCF into the magnon and soliton