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## Dynamics of the one-dimensional spin-1 Heisenberg antiferromagnet with exchange and single-site anisotropy

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The  $T=0$  dynamical properties of the one-dimensional  $s=1$  XXZ model with an additional single-site term are investigated by means of the recursion method. The dynamic structure factors  $S_{\mu\mu}(q=\pi, \omega)$ ,  $\mu=x, z$  bear the characteristic signatures of several different phase transitions. In the  $s=1$  Heisenberg antiferromagnet, the intrinsic linewidth (at fixed  $q$ ) of  $S_{\mu\mu}(q, \omega)$  is larger for small  $q$  than for  $q$  near  $\pi$ , in contrast to well-established results for the corresponding  $s=\frac{1}{2}$  model.

Spin chains with quantum number  $s=1$  have been the object of sustained intense study ever since 1983, when Haldane<sup>1</sup> first predicted the existence of a nonmagnetic phase with an excitation gap for the isotropic Heisenberg antiferromagnet. That research activity has led to a broad consensus on the main features, and many intricate details of the  $T=0$  phase diagrams pertaining to several model Hamiltonians involving spin-1 chains. The prototype among them is the Heisenberg antiferromagnet with exchange and single-site anisotropies,

$$H = \sum_{l=1}^N [J(S_l^x S_{l+1}^x + S_l^y S_{l+1}^y) + J_z S_l^z S_{l+1}^z + D(S_l^z)^2]. \quad (1)$$

Within the domain  $0 \leq J_z/J \leq 2$ ,  $0 \leq D/J \leq 2$  considered here for the two anisotropy parameters, a total of four distinct  $T=0$  phases have been identified:<sup>2-5</sup> (i) A Néel phase ( $N$ ) with antiferromagnetic long-range order in  $z$  direction is realized for sufficiently large  $J_z/J$ . (ii) A singlet phase ( $S$ ) characterized by a nondegenerate ground state, and an excitation gap exists for large  $D/J$ . (iii) A critical phase ( $C$ ) with algebraically decaying in-plane correlation function  $\langle S_l^x S_{l+n}^x \rangle$  is present for sufficiently small  $J_z/J$  and  $D/J$ . (iv) Contiguous to these three phases is the phase ( $H$ )—the one first predicted by Haldane. Like ( $S$ ), it is characterized by a nonmagnetic singlet ground state with an excitation gap.<sup>6</sup> The ground state is critical on the boundaries of ( $H$ ). The ( $C/H$ ) transition is of the Kosterlitz–Thouless type, and the ( $N/H$ ) transition is of the 2D-Ising variety. Both transitions are specified by a single set of critical exponents for the entire phase boundary, except at the endpoints. The critical exponents of the ( $S/H$ ) transition, by contrast, vary continuously along the phase boundary.

What is the characteristic signature of the four phases, and the impact of the three transitions on the  $T=0$  dynamic structure factors  $S_{\mu\mu}(q, \omega)$ , defined as the Fourier transforms of the space-time correlation functions  $\langle S_l^\mu(t) S_{l+n}^\mu \rangle$ ,  $\mu=x, z$ ? The first goal of this study is to investigate this important

question with an application of the recursion method. The second goal will be a study of line shapes of  $S_{\mu\mu}(q, \omega)$  for an experimentally relevant situation.

The recursion method, which, in the present context, is based on an orthogonal expansion of the wave function  $|\psi_q^\mu(t)\rangle = S_q^\mu(-t)|\phi_0\rangle$ ,  $S_q^\mu = N^{-1/2} \sum_l e^{iql} S_l^\mu$ , yields (after several intermediate steps)<sup>7,8</sup> a sequence of continued-fraction coefficients  $\Delta_1^{\mu\mu}(q), \Delta_2^{\mu\mu}(q), \dots$ , for the relaxation function,

$$c_0^{\mu\mu}(q, z) = \frac{1}{z + \frac{\Delta_1^{\mu\mu}(q)}{z + \frac{\Delta_2^{\mu\mu}(q)}{z + \dots}}}, \quad (2)$$

from which the  $T=0$  dynamic structure factor can be inferred as

$$S_{\mu\mu}(q, \omega) = 4 \langle S_q^\mu S_{-q}^\mu \rangle \Theta(\omega) \lim_{\epsilon \rightarrow 0} \Re [c_0^{\mu\mu}(q, \epsilon - i\omega)]. \quad (3)$$

The finite-size ground-state wave function  $|\phi_0\rangle$  must be computed up front. We use the conjugate-gradient method for that task.<sup>9</sup>

Despite the nontrivial  $N$  dependence of  $|\phi_0\rangle$  in the present application, the first  $K \approx N/2$  coefficients  $\Delta_1^{\mu\mu}(q), \dots, \Delta_K^{\mu\mu}(q)$  are, at most, *weakly* size dependent. They reflect key properties of  $S_{\mu\mu}(q, \omega)$  for the infinite system more faithfully than the subsequent coefficients, which depend *strongly* on  $N$ . Our continued-fraction analysis uses the nearly size-independent coefficients (i) for the detection of dynamically relevant excitation gaps and (ii) for the determination of the spectral-weight distribution in  $S_{\mu\mu}(q, \omega)$ .

As is typical in quantum many-body dynamics, the nearly size-independent sequences  $\Delta_k^{\mu\mu}(q)$ ,  $k=1, \dots, K$ , obtained here grow linearly with  $k$ , on average, and exhibit one or several patterns that translate into specific properties of  $S_{\mu\mu}(q, \omega)$  related to the type of ordering, the presence of excitation gaps, the size of bandwidths, and the exponents of infrared singularities. The techniques of analysis for these properties have been described in previous or concurrent ap-

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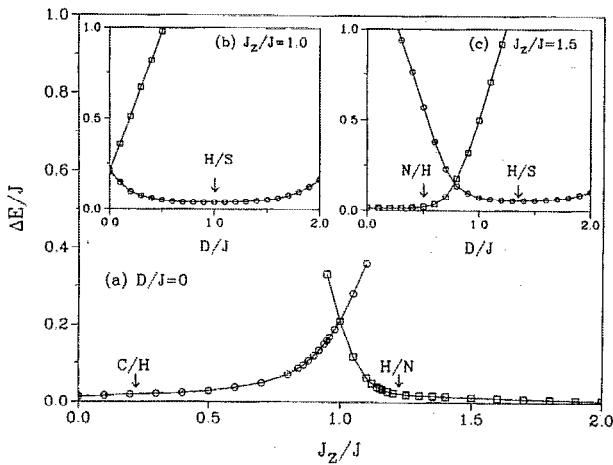


FIG. 1. Dynamically relevant excitation gaps for operators  $S_\pi^x$  (circles) and  $S_\pi^z$  (squares) along three lines in the parameter space of the Hamiltonian (1). The gaps are derived from  $K=6$  nearly size-independent continued-fraction coefficients  $\Delta_k^{\mu}(\pi)$ ,  $k=1, \dots, K$  computed by means of the recursion method from the  $N=12$  ground-state wave function. The vertical arrows indicate the locations where the three lines in parameter space cross phase boundaries.

plications of the recursion method to the 1D and 2D  $s=\frac{1}{2}$   $XXZ$  models<sup>7,8</sup> and the 1D spin- $s$   $XYZ$  model.<sup>10</sup>

For our first task, which is to map out the rather complex phase diagram of (1) in the given parameter range, we choose an operator (in our case  $S_q^\mu$  with  $q=\pi$  and  $\mu=x, z$ ) which we know or expect to represent the critical fluctuations along a specified phase boundary. The method of determining the dynamically relevant excitation gap for that operator involves the matching of the nearly size-independent coefficients  $\Delta_1^{\mu}(q), \dots, \Delta_K^{\mu}(q)$ , with the first  $K$  coefficients  $\tilde{\Delta}_1(\Omega), \dots, \tilde{\Delta}_K(\Omega)$  of a suitable model dynamic structure factor that has a gap of size  $\Omega$ .<sup>8</sup> Since the matching criterion is not unique we cannot expect to obtain from that analysis accurate values for the gap sizes. Nevertheless, it proves to be a reliable indicator for the identification of phase boundaries and the dynamical variables that are subject to critical fluctuations.

For this short work, we have carried out the gap analysis along three lines in  $(J_z/J, D/J)$  space. In Fig. 1(a) we have plotted the  $J_z/J$  dependence for fixed  $D/J=0$  of the excitation gaps which are dynamically relevant for the operators  $S_\pi^x$  (circles) and  $S_\pi^z$  (squares). At  $J_z/J=0$ , our analysis yields a  $S_\pi^x$  gap very close to zero, and it remains near zero over some range of  $J_z/J$  values, reflecting the extended critical phase (C). The large  $S_\pi^z$  gap in that region indicates that the out-of-plane fluctuations are not critical. Even past the transition to the Haldane phase, marked (C/H) in Fig. 1(a), the  $S_\pi^x$  gap opens only very slowly, which is typical near a Kosterlitz–Thouless-type phase boundary. This is in marked contrast to the more rapid closing of the  $S_\pi^z$  gap at the other end of the Haldane phase. The (H/N) transition marks the onset of antiferromagnetic long-range order in the  $z$  direction. The large  $S_\pi^x$  gap near the phase boundary confirms Haldane's prediction<sup>1</sup> that the in-plane fluctuations have no part in that transition.

For the second line in parameter space [see Fig. 1(b)], we keep the exchange parameter fixed at  $J_z/J=1$  and vary the single-site parameter  $D/J$ . At  $D/J=0$ , which is equivalent to the midpoint of line (a), the  $S_\pi^z$  gap starts out nonzero and grows with increasing  $D/J$ , which reflects the fact that low-frequency out-of-plane fluctuations are more and more suppressed as the easy-plane anisotropy becomes stronger. The  $S_\pi^x$  gap, by contrast, has a decreasing trend. Starting from the same value at  $D/J=0$ , it reaches a minimum near zero at  $D/J \approx 1.0$  and then grows again. The minimum marks the (H/S) transition between two nonmagnetic phases, where only the staggered in-plane fluctuations become critical.

Now we shift the line  $0 \leq D/J \leq 2$  in parameter space from  $J_z/J=1$  [Fig. 1(b)] to  $J_z/J=1.5$  [Fig. 1(c)]. At  $D/J=0$  the system is in the Néel phase. Here the  $S_\pi^x$  gap is large, reflecting the transverse spin waves of a uniaxial antiferromagnet, whereas the  $S_\pi^z$  gap is effectively zero, reflecting the twofold degeneracy of the ground state associated with antiferromagnetic ordering. As  $D/J$  increases from zero, the  $S_\pi^z$  gap stays near zero up to the (N/H) phase boundary at  $D/J \approx 0.5$ , where it starts to increase very rapidly with no further change in course. The  $S_\pi^x$  gap decreases from some large value as  $D/J$  increases from zero. It goes through a minimum near zero at  $D/J \approx 1.7$ , marking, as in Fig. 1(b), the (H/S) transition, now shifted to a higher value of single-site anisotropy, in agreement with the broadly accepted picture.<sup>2-6</sup>

The significance of the results displayed in Fig. 1 is that they have been derived entirely from the ground-state wave function of a chain with just  $N=12$  spins. It is certainly surprising that the spectral signatures of a rather complex phase diagram are so clearly encoded in that quantity and that this information is so easily retrievable.

The same type of gap analysis carried out for the  $q$  dependence of the operator  $S_q^\mu$  yields the dispersion of the lowest branch of excitations which is dynamically relevant for  $S_{\mu\mu}(q, \omega)$ . Toward our second goal we reconstruct the dynamic structure factor itself via (3) from expression (2) with coefficients  $\Delta_1^{\mu}(q), \dots, \Delta_K^{\mu}(q)$  and a termination function tailored, such as to extrapolate the recognizable pattern of the first  $K$  coefficients. A detailed account of the reconstruction has been reported in Ref. 8. Here we must limit the discussion to a couple of specific issues: What is the main difference in line shape between the functions  $S_{\mu\mu}(q, \omega)$  of the  $s=1$  Heisenberg antiferromagnet and its  $s=\frac{1}{2}$  counterpart, and what is the impact of a small easy-plane single-site anisotropy on the peak positions and line shapes in the  $s=1$  case?

Figure 2(a) shows the reconstructed (normalized) dynamic structure factor  $\tilde{S}_{\mu\mu}(q, \omega) \equiv S_{\mu\mu}(q, \omega) / \langle S_q^\mu S_{-q}^\mu \rangle$  at  $q=\pi/6$  and  $q=5\pi/6$  for the 1D  $s=1$  Heisenberg antiferromagnet. For both wave numbers, the function consists of a single peak with nonzero intrinsic linewidth. This is in strong contrast to the results obtained from truncated continued fractions<sup>11</sup> or equivalent procedures,<sup>12</sup> which are sums of  $\delta$  functions, often broadened into Lorentzians for graphical representation.

We note two main differences between the results of Fig.

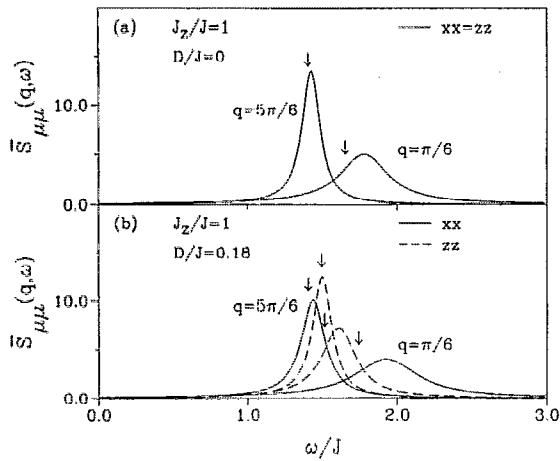


FIG. 2. Normalized dynamic structure factor  $S_{\mu\mu}(q, \omega) / (S_q^\mu S_{-q}^\mu)$  at  $T=0$  of (a) the 1D  $s=1$  Heisenberg antiferromagnet and (b) the same model with an additional easy-plane single-site anisotropy,  $D/J=0.18$ . We show results for  $\mu=x, z$ , and  $q=\pi/6, 5\pi/6$ . They have been derived from  $K=6$  continued-fraction coefficients  $\Delta_k^{\mu\mu}(q), k=1, \dots, K$  extracted from the  $N=12$  ground-state wave function combined with the continued-fraction analysis described in Ref. 8. The arrow near the peak of each curve indicates the energy of the lowest excitation with nonzero matrix element in  $S_{\mu\mu}(q, \omega)$  of the  $N=12$  chain.

2(a) and the corresponding results of the  $s=\frac{1}{2}$  model (see Ref. 8): (a) the peak positions at wave numbers  $q$  and  $\pi-q$  are the same for  $s=\frac{1}{2}$ , but differ substantially for  $s=1$ . The symmetric dispersion of the  $s=\frac{1}{2}$  chain is exactly known, and the asymmetric dispersion of the  $s=1$  chain has been well established by extensive numerical diagonalizations.<sup>11,12</sup> (b) The linewidth is known to increase monotonically with increasing  $q$  in the  $s=\frac{1}{2}$  case,<sup>8,13</sup> but in Fig. 2(a) the  $s=1$  result at small  $q$  has a considerably larger linewidth than the one at  $q$  near  $\pi$ . Our  $s=1$  results are consistent with the findings of Refs. 11 and 12 that the spectral weight in  $S_{\mu\mu}(q, \omega)$  is dominated by a single  $\delta$  function at  $q$  near  $\pi$ , but less so at small  $q$ . The opposite trends of line broadening in the  $s=\frac{1}{2}$  and  $s=1$  chains may be understood by interpreting the observable excitations as composites of different kinds of elementary states.

The presence of some easy-plane anisotropy,  $D/J=0.18$ , alters the functions  $S_{\mu\mu}(\pi/6, \omega)$  and  $S_{\mu\mu}(5\pi/6, \omega)$ , as shown in Fig. 2(b). In-plane ( $xx$ ) and out-of-plane ( $zz$ ) fluctuations are now represented by separate peaks. At small  $q$ , the in-plane peak has moved up and the out-of-plane peak down. At small  $\pi-q$ , they have moved in opposite direc-

tions. The anisotropy causes an increase in in-plane linewidths. The peak positions of the reconstructed functions  $S_{\mu\mu}(5\pi/6, \omega)$  shown in Fig. 2 are in good agreement with the energies of the lowest-lying dynamically relevant excitation of a chain with  $N=12$  spins. The latter, quoted from Ref. 12, are indicated by arrows in Fig. 2. However, for  $q=\pi/6$  the peaks lie significantly higher than the lowest  $N=12$  excitation.

The significance of the point  $(J_z/J=1, D/J=0.18)$  in the parameter space of Hamiltonian (1) is its physical realization by the quasi-1D magnetic compound  $\text{Ni}(\text{C}_2\text{H}_8\text{N}_2)_2\text{NO}_2\text{ClO}_4$  (NENP). A recent inelastic neutron scattering study on that compound<sup>14</sup> observes well-defined resonances for  $0.3\pi \leq q \leq \pi$ , including  $q=5\pi/6$ , where our result predicts a peak with small but nonzero linewidth. At smaller wave numbers including  $q=\pi/6$ , the resonance in the experiment has disappeared in a broad background intensity. Here our analysis predicts a broad signal, which, when multiplied by the very small integrated intensity, becomes indeed undetectable for all practical purposes.

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