

## Limitations of spin-wave theory in $T=0$ spin dynamics

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The  $T=0$  dynamics of a family of one-dimensional quantum spin systems with fully ordered (ferromagnetic or spin-flop) ground states is investigated. By rigorous calculations, it is demonstrated that the  $T=0$  dynamic structure factor is, in general, not a  $\delta$  function as predicted by linear spin-wave theory but characterized by more complicated structures with nonzero linewidths. The exact result approaches the spin-wave result in the classical limit  $s \rightarrow \infty$ . The results of this study demonstrate how quantum effects may invalidate spin-wave theory even in the presence of saturated magnetic long-range order. Hence the failure of spin-wave theory is not necessarily linked to the absence or strong reduction of long-range order typical for one-dimensional quantum spin systems. The unreliability of spin-wave theory has therefore to be suspected also for the dynamics of three-dimensional quantum spin systems where the long-range order is always strong at  $T=0$ .

### I. INTRODUCTION

Spin-wave theory<sup>1,2</sup> is based on the expansion of any given quantum spin Hamiltonian  $H$  in terms of boson operators. In the linear spin-wave (LSW) approximation, all terms but the harmonic term are neglected. Anharmonic corrections may then be treated as perturbations. Optimal circumstances for the use of LSW theory are found in situations where the ground state of  $H$  is ferromagnetic. The LSW approximation then gives the exact ground state. The excited states of  $H$ , on the other hand, are replaced by noninteracting spin-wave states (magnons), which obey Bose statistics.<sup>3</sup> At  $T=0$ , only the one-magnon states contribute to the dynamic structure factor<sup>4</sup>

$$S_{\mu\mu}(\vec{q}, \omega) \equiv N^{-1} \sum_{i,j} \exp[-i\vec{q} \cdot (\vec{R}_i - \vec{R}_j)] \times \int_{-\infty}^{+\infty} dt e^{i\omega t} [\langle S_i^\mu(t) S_j^\mu \rangle - \langle S_i^\mu \rangle \langle S_j^\mu \rangle]. \quad (1)$$

Hence in the LSW approximation,  $S_{\mu\mu}(\vec{q}, \omega)$  as a function of  $\omega$  for fixed  $\vec{q}$  has the characteristic form

$$S_{\mu\mu}(\vec{q}, \omega) = 2\pi \Phi_{\mu\mu}(\vec{q}) \delta(\omega - \epsilon(\vec{q})), \quad (2)$$

where  $\epsilon(\vec{q})$  is the dispersion of the one-magnon states and  $\Phi_{\mu\mu}(\vec{q})$  is the integrated intensity.

Spin-wave theory is a major theoretical tool with a wide range of applications in the study of magnetism as a cooperative phenomenon.<sup>1</sup> However, the reliability and accuracy of theoretical predictions based on spin-wave theory cannot, in general, be tested because exact results for realistic magnetic model Hamiltonians are scarce. This is particularly the case for applications in spin dynamics where spin-wave theory and, in particular, the LSW approximation are widely used. In fact, rigorous results for the dynamics of quantum spin systems are limited to one dimension (1D).<sup>5</sup> In 1D, the limitations of spin-wave theory have indeed been demonstrated.<sup>6</sup> However, the reason for its failure has been attributed to the fact

that in the ground state of 1D quantum spin systems, there are strong quantum fluctuations which reduce the magnitude of the order parameter considerably below its saturation value or, in some cases, destroy long-range order altogether.

The 1D  $s = \frac{1}{2}$  XXZ model

$$H = -J \sum_{l=1}^N (S_l^x S_{l+1}^x + S_l^y S_{l+1}^y + \Delta S_l^z S_{l+1}^z) \quad (3)$$

is a typical example of a model which reflects this connection between the degree of ordering in the ground state and the accuracy of the LSW approximation: For  $\Delta \geq 1$ , the ground state of (3) is ferromagnetic and the  $T=0$  dynamic structure factor has the form (2); LSW theory is exact. For  $\Delta < 1$ , on the other hand, the ground state is either not ordered at all ( $-1 \leq \Delta < 1$ ) or only partially ordered ( $-\infty < \Delta < -1$ ). In both cases, it is well established that the LSW prediction fails;  $S_{\mu\mu}(q, \omega)$  has a much more complex structure than given by (2). In the limit  $\Delta \rightarrow -\infty$ , the order parameter is gradually saturated and  $S_{\mu\mu}(q, \omega)$  again approaches the form (2). All this is in support of the widespread belief that the LSW prediction for the dynamic structure factor becomes very accurate if only the reduction of the order parameter (called spin reduction) caused by thermal or quantum fluctuations is very small. This belief, in turn, has led to much confidence in the LSW theory for three-dimensional (3D) magnets because of the experimental and theoretical evidence that there the spin reduction at low  $T$  is usually very small.<sup>7</sup>

In this paper we demonstrate that the limitations of LSW theory for the  $T=0$  dynamics of quantum spin systems are not necessarily linked to the presence of strong quantum fluctuations causing spin reduction in the ground state. We investigate the  $T=0$  dynamics of a family of 1D quantum spin systems with fully ordered (ferromagnetic or spin-flop) ground states<sup>8</sup> and show by rigorous calculations that the  $T=0$  dynamic structure factor differs dramatically from the LSW prediction. This implies that the failure of LSW theory is related, more directly, to the nonlinear nature of the underlying equa-

tions of motion, i.e., to the anharmonic correction terms in  $H$  which are neglected in the LSW approximation.<sup>9</sup> Since these nonlinearities are also present in higher-dimensional systems, there is no reason *a priori* to believe that their effects which are manifest in the exactly solvable 1D case should be less pronounced in its two-dimensional (2D) and 3D counterparts.

## II. THE ANISOTROPIC XY MODEL

In this section we investigate the adequacy of LSW theory for a family of quantum spin system with the properties of (i) having a fully ordered ground state and (ii) being amenable to rigorous calculations. The system under consideration is the 1D anisotropic XY model in a magnetic field  $h$  described by the Hamiltonians

$$H_{\pm} = \pm J \sum_{l=1}^N [(1+\gamma)S_l^x S_{l+1}^x + (1-\gamma)S_l^y S_{l+1}^y] - h \sum_{l=1}^N S_l^z, \quad (4)$$

with  $0 \leq \gamma \leq 1$ ,  $J > 0$ . Here  $H_+$  characterizes the XY anti-ferromagnet and  $H_-$  the XY ferromagnet. The canonical transformation

$$U = \exp \left[ i\pi \sum_{l=1}^N l S_l^z \right], \quad (5)$$

which has the effect of rotating every other spin by  $180^\circ$  about the  $z$  axis, maps the two models onto one another (we consider only even  $N$ )<sup>10</sup>:

$$U H_+ U^{-1} = H_- . \quad (6)$$

Hence, given the eigenfunctions  $|\lambda\rangle_+$ ,  $\lambda=1,2,\dots$ ,  $(2s+1)^N$ , and energy eigenvalues  $E_\lambda^+$  of  $H_+$ , the eigenfunctions of  $H_-$  are obtained as  $|\lambda\rangle_- = U |\lambda\rangle_+$  having the same energies  $E_\lambda^- = E_\lambda^+$ .

For  $s = \frac{1}{2}$ , the ground-state properties of (4) are exactly known.<sup>11</sup> This is not the case for  $s > \frac{1}{2}$ . Only recently it has been shown for arbitrary  $s$  that at the special value

$$h = h_N = 2sJ(1-\gamma^2)^{1/2} \quad (7)$$

of the magnetic field, the ground state of  $H_+$  can be expressed as a direct product

$$|G\rangle_+ = |\theta_1^+\rangle \otimes |\theta_2^+\rangle \otimes \cdots \otimes |\theta_N^+\rangle, \quad \theta_l^+ = (-1)^l \theta \quad (8)$$

of single-site states<sup>12,13</sup>

$$S_{\mathbf{z}}(q, \omega) = \frac{1}{2} \int_0^\pi dk [1 - f(k, q)] \delta(\omega - \epsilon(k, q)), \quad (13a)$$

$$\epsilon(k, q) = J \{ [\tilde{h} + \cos(k - q/2)]^2 + \gamma^2 \sin^2(k - q/2) \}^{1/2} + \{ [\tilde{h} + \cos(k + q/2)]^2 + \gamma^2 \sin^2(k + q/2) \}^{1/2}, \quad (13b)$$

$$f(k, q) = \frac{[\tilde{h} + \cos(k - q/2)][\tilde{h} + \cos(k + q/2)] - \gamma^2 \sin(k - q/2) \sin(k + q/2)}{\{ [\tilde{h} + \cos(k - q/2)]^2 + \gamma^2 \sin^2(k - q/2) \}^{1/2} \{ [\tilde{h} + \cos(k + q/2)]^2 + \gamma^2 \sin^2(k + q/2) \}^{1/2}}, \quad (13c)$$

with  $\tilde{h} = h/J$ . For  $h = h_N$ , the evaluation of this expression is very simple<sup>16</sup>:

$$S_{\mathbf{z}}(q, \omega) = \frac{\gamma^2 [4J^2(1-\gamma^2)\cos^2(q/2) - (\omega - 2J)^2]}{1-\gamma^2 [\omega - 2J \sin^2(q/2)]^2 + J^2 \gamma^2 \sin^2 q} \theta[4J^2(1-\gamma^2)\cos^2(q/2) - (\omega - 2J)^2]. \quad (14)$$

$$|\theta\rangle = \sum_{m=-s}^{+s} \left[ \frac{(2s)!}{(s+m)!(s-m)!} \right]^{1/2} \left[ \cos \frac{\theta}{2} \right]^{s+m} \times \left[ \sin \frac{\theta}{2} \right]^{s-m} |m\rangle, \quad (9a)$$

$$\cos \theta = [(1-\gamma)/(1+\gamma)]^{1/2}. \quad (9b)$$

Here  $|m\rangle$  are the  $2s+1$  eigenfunctions of  $\bar{S}_l^z$  and  $S_l^z$  with eigenvalues  $s(s+1)$  and  $m$ , respectively. The ground state  $|G\rangle_-$  of  $H_-$  is then<sup>14</sup>

$$|G\rangle_- = U |G\rangle_+ = |\theta_1^-\rangle \otimes |\theta_2^-\rangle \otimes \cdots \otimes |\theta_N^-\rangle, \quad \theta_l^- = \theta = \text{const}. \quad (10)$$

$|G\rangle_+$ , the ground state of  $H_+$ , is a spin-flop state with sublattice magnetizations

$$\vec{M}_+^A \equiv \langle G | \vec{S}_{2l-1} | G \rangle_+ = (-s \sin \theta, 0, s \cos \theta), \quad (11a)$$

$$\vec{M}_+^B \equiv \langle G | \vec{S}_{2l} | G \rangle_+ = (s \sin \theta, 0, s \cos \theta), \quad (11b)$$

and  $|G\rangle_-$ , the ground state of  $H_-$ , is ferromagnetic in the sense that all spins are aligned. The magnetization of  $|G\rangle_-$ ,

$$\vec{M}_- \equiv \langle G | \vec{S}_l | G \rangle_- = (s \sin \theta, 0, s \cos \theta), \quad (12)$$

is saturated as are the sublattice magnetizations of  $|G\rangle_+$ . In these states, which we call fully ordered, the quantum fluctuations are minimal; they are reflected only in the fact that the magnitude of the sublattice magnetizations  $\vec{M}_+^A, \vec{M}_+^B$  and of the magnetization  $\vec{M}_-$ , all given by  $|\langle \vec{S}_l \rangle| = s$ , falls short of the total "spin length"  $\sqrt{s(s+1)}$ . We now proceed to study the properties of the  $T=0$  dynamic structure factors  $S_{\mu\mu}(q, \omega)$ ,  $\mu=x, y, z$ , of this system, where quantum effects will be much more pronounced.

### A. $S_{\mathbf{z}}(q, \omega)$ for $s = \frac{1}{2}$

An implication of (6) is that the dynamic structure factor  $S_{\mathbf{z}}(q, \omega)$  is the same for  $H_+$  and  $H_-$ . For the  $s = \frac{1}{2}$  case we are in the fortunate situation that the importance of quantum fluctuations can be demonstrated by explicit rigorous calculations: The time-dependent spin-correlation function  $\langle S_l^z(t) S_{l+R}^z \rangle$  of (4) with  $s = \frac{1}{2}$  and  $\gamma, h$  arbitrary can be expressed as a density-density correlation function of a system of noninteracting fermions.<sup>15</sup> The corresponding expression for the dynamic structure factor at  $T=0$  reads

$S_{\mathbf{z}\mathbf{z}}(q, \omega)$  is nonzero in the two-parameter continuum

$$|\omega - 2J| < 2J(1 - \gamma^2)^{1/2} \cos(q/2)$$

of the  $(q, \omega)$  plane as illustrated in Figs. 1 and 2. For fixed  $q$ ,  $S_{\mathbf{z}\mathbf{z}}(q, \omega)$  is characterized by a rounded peak close to the lower boundary and a tail out to the upper boundary. As  $q$  approaches  $\pi$ , the peak rises steeply while its width diminishes.

We note that despite the realization of a fully ordered ground state, the dynamic structure factor (14) differs a great deal from the LSW prediction which is<sup>12</sup>

$$S_{\mathbf{z}\mathbf{z}}^{\text{sw}}(q, \omega) = 2\pi[s\gamma/(1+\gamma)]\delta(\omega - \epsilon_{\text{sw}}(q)), \quad (15a)$$

$$\epsilon_{\text{sw}}(q) = 2sJ[(1+\gamma) - (1-\gamma)\cos q]. \quad (15b)$$

The spin-wave (sw) energy, also shown in Fig. 1, does not coincide with the peak frequency of (14) except at  $q = \pi$ . Here, the two expressions (14) and (15) are equivalent.

### B. $S_{\mathbf{z}\mathbf{z}}(q, \omega)$ for arbitrary $s$

Although we know the exact ground-state wave functions of (4) for arbitrary  $s$ , we are unable to derive an exact expression for the  $T=0$  dynamic structure factor for

$$K_{\mathbf{z}\mathbf{z}}^{(1)}(q) = 2s^2J[\gamma/(1+\gamma)][(1+\gamma) - (1-\gamma)\cos q], \quad (17)$$

$$K_{\mathbf{z}\mathbf{z}}^{(3)}(q) = 4J^3[\gamma/(1+\gamma)]\{2s^4[(1+\gamma) - (1-\gamma)\cos q]^3$$

$$+ 2s^3\gamma(1-\gamma)(1+\cos q)[2(1+\gamma) - (1-\gamma)\cos q] - s^2\gamma^2(1-\gamma)(1+\cos q)\}. \quad (18)$$

From (8) or (10), we can also calculate the integrated intensity

$$\Phi_{\mathbf{z}\mathbf{z}}(q) = K_{\mathbf{z}\mathbf{z}}^{(0)}(q) \equiv \int_0^\infty \frac{d\omega}{2\pi} S_{\mathbf{z}\mathbf{z}}(q, \omega) = \sum_R e^{-iqR} (\langle S_i^z S_{i+R}^z \rangle - \langle S_i^z \rangle \langle S_{i+R}^z \rangle) = s \frac{\gamma}{1+\gamma}. \quad (19)$$

For  $s = \frac{1}{2}$ , the sum rules (17)–(19) are verified by the corresponding frequency moments of (14). Note that the spin-wave result (15) also satisfies (17) and (19) for arbitrary  $s$ , but it does not satisfy the sum rule (18).  $K_{\mathbf{z}\mathbf{z}}^{(3)}(q)$  has a nontrivial  $s$  dependence which comes from correlation functions in (16) containing noncommuting spin operators. In the classical limit  $s \rightarrow \infty$ , all terms in (18) except those multiplied by the largest power of  $s$  are negli-

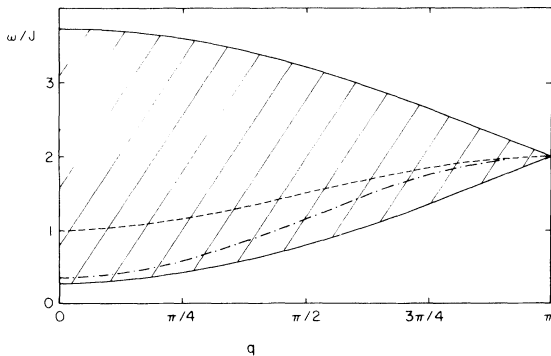


FIG. 1. Spectrum of the dynamic structure factor  $S_{\mathbf{z}\mathbf{z}}(q, \omega)$  at  $T=0$  of  $H_{\pm}$  for  $s = \frac{1}{2}$ ,  $h = h_N$ ,  $\gamma = \frac{1}{2}$ . The shaded area corresponds to  $|\omega - 2J| \leq 2J(1 - \gamma^2)^{1/2} \cos(q/2)$ , where  $S_{\mathbf{z}\mathbf{z}}(q, \omega)$  is nonzero.  $S_{\mathbf{z}\mathbf{z}}(q, \omega)$  as a function of  $\omega$  for fixed  $q$  has a peak at the energy characterized by the dot-dashed line. The dashed line denotes the spin-wave energy Eq. (15b).

$s > \frac{1}{2}$ . Nevertheless, we can deduce valuable information on  $S_{\mathbf{z}\mathbf{z}}(q, \omega)$  from (8)–(10).

In a recent paper<sup>17</sup> an infinite set of sum rules has been derived for the dynamic structure factor of quantum spin chains. The major result is that the  $n$ th ( $n = 1, 3, 5, \dots$ ) frequency moment of the  $T=0$  dynamic structure factor  $S_{\mu\mu}(q, \omega)$  is a polynomial in  $\cos q$  of degree  $n$  with coefficients determined by static  $m$ -point correlation functions<sup>18</sup> ( $m = 1, 2, \dots, n + 1$ ):

$$K_{\mu\mu}^{(n)}(q) \equiv \int_0^\infty \frac{d\omega}{2\pi} \omega^n S_{\mu\mu}(q, \omega) = \sum_{m=0}^n A_m^n \cos^m q, \quad n = 1, 3, 5, \dots \quad (16a)$$

$$A_m^n = \sum_j b_j^{(m)} \langle S_{l_0}^{\beta_0} S_{l_1}^{\beta_1} \dots S_{l_m}^{\beta_m} \rangle,$$

$$l_0 \leq l_1 \leq \dots \leq l_m, \quad l_m - l_0 \leq n. \quad (16b)$$

For the system under investigation the coefficients  $A_m^n$  can be evaluated explicitly using the exact ground-state wave functions (8) or (10). The results for  $n = 1, 3$  read

$$K_{\mathbf{z}\mathbf{z}}^{(1)}(q) = 2s^2J[\gamma/(1+\gamma)][(1+\gamma) - (1-\gamma)\cos q], \quad (17)$$

$$K_{\mathbf{z}\mathbf{z}}^{(3)}(q) = 4J^3[\gamma/(1+\gamma)]\{2s^4[(1+\gamma) - (1-\gamma)\cos q]^3 + 2s^3\gamma(1-\gamma)(1+\cos q)[2(1+\gamma) - (1-\gamma)\cos q] - s^2\gamma^2(1-\gamma)(1+\cos q)\}. \quad (18)$$

gible.  $K_{\mathbf{z}\mathbf{z}}^{(3)}(q)$  is then equal to the third frequency moment of the spin-wave result (15).

Thus the  $T=0$  dynamic structure factor  $S_{\mathbf{z}\mathbf{z}}(q, \omega)$  of the model (4) at  $h = h_N$ , which has the quasiclassical (fully or-

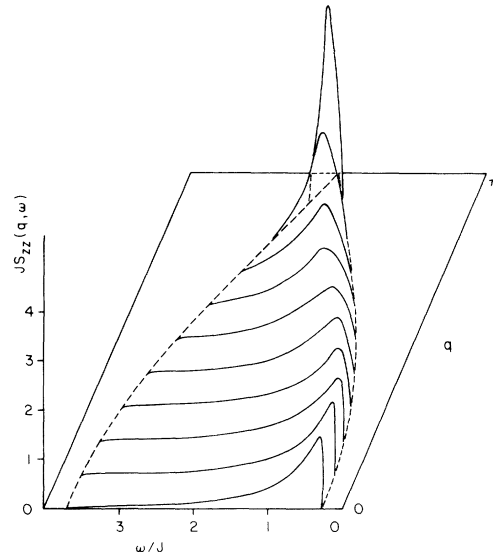


FIG. 2. Dynamic structure factor  $S_{\mathbf{z}\mathbf{z}}(q, \omega)$  at  $T=0$  of  $H_{\pm}$  for  $s = \frac{1}{2}$ ,  $h = h_N$ ,  $\gamma = \frac{1}{2}$ , as a function of frequency for wave numbers  $q = n\pi/10$ ,  $n = 0, 1, \dots, 9$ .

dered) ground state (8) or (10), is nontrivial for all finite  $s$ . The spin-wave result (15) is recovered in the classical limit after rescaling of the energy unit  $J$ :  $s \rightarrow \infty$ ,  $J \rightarrow 0$  such that  $J' = 2Js$  stays constant.

Using the exact sum rules (17)–(19) we may define the following two quantities:

$$\Omega_z(q) = \langle \omega \rangle_z / 2s, \quad \Gamma_z(q) = (\langle \omega^3 \rangle_z - \langle \omega \rangle_z^3)^{1/3} / 2s, \quad (20)$$

with

$$\langle \omega^n \rangle_z = K_z^{(n)}(q) / K_z^{(0)}(q). \quad (21)$$

In a situation where  $\Gamma_z(q) \ll \Omega_z(q)$  holds, the spectral weight is concentrated in a relatively narrow frequency range for fixed  $q$ . Then,  $\Omega_z(q)$  can be interpreted as a renormalized “line frequency” and  $\Gamma_z(q)$  as a measure for the corresponding “linewidth.” We have

$$\begin{aligned} \Omega_z(q) &= J[(1+\gamma) - (1-\gamma)\cos q], \quad (22) \\ \Gamma_z(q) &= Js^{-1/3} \{ \gamma(1-\gamma)(1+\cos q) \\ &\quad \times [2(1+\gamma) - (1-\gamma)\cos q - \gamma/2s] \}^{1/3}. \quad (23) \end{aligned}$$

Evidently,  $2s\Omega_z(q)$  coincides with the spin-wave frequency (15b). The  $q$  dependence of both  $\Omega_z$  and  $\Gamma_z$  are plotted in Fig. 3 for various  $s$ .  $\Gamma_z(q)$  vanishes at  $q = \pi$  irrespective of the quantum number  $s$ , indicating that  $S_{zz}(\pi, \omega)$  is a  $\delta$  function for any  $s$ . The condition  $\Gamma_z \ll \Omega_z$  is generally not satisfied for  $s \lesssim \frac{5}{2}$ , i.e., for low-spin quantum numbers typically encountered in real magnets. Hence the physical interpretation of the dynamic structure factor cannot be interpreted in terms of “line frequency” and “linewidth” unless  $s$  is fairly large.

### C. A remark on $S_{xx}(q, \omega)$ and $S_{yy}(q, \omega)$

For  $s = \frac{1}{2}$ ,  $\langle S_i^x(t)S_{i+R}^x \rangle$  and  $\langle S_i^y(t)S_{i+R}^y \rangle$  are again correlation functions of a noninteracting fermion system. In contrast to  $\langle S_i^z(t)S_{i+R}^z \rangle$ , however, they are related to fermion correlation functions involving, in general, an infinite number of field operators. In fact,  $\langle S_i^x(t)S_{i+R}^x \rangle$  and  $\langle S_i^y(t)S_{i+R}^y \rangle$  could be expressed in terms of infinite block Toeplitz determinants for arbitrary  $\gamma, h$ .<sup>19</sup> No explicit expressions for  $S_{xx}(q, \omega)$  and  $S_{yy}(q, \omega)$  have been evaluated. No results exist for  $s > \frac{1}{2}$ .

From the exactly known ground-state wave functions (8)–(10) at  $h = h_N$ , we can derive explicit expressions for

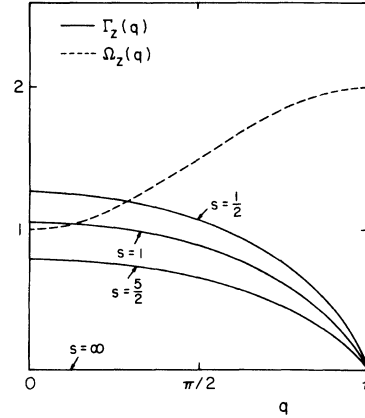


FIG. 3. Linewidths  $\Gamma_z(q)$  (solid curves) and renormalized line frequencies  $\Omega_z(q)$  (dashed curve) as defined in Eqs. (22) and (23) for the  $T=0$  dynamic structure factor  $S_{zz}(q, \omega)$  of the anisotropic XY model in a magnetic field  $h = 2sJ(1-\gamma^2)^{1/2}$  for various  $s$  and  $\gamma = \frac{1}{2}$ . Note that  $\Omega_z(q)$  is not  $s$  dependent.

the transverse components of the sum rules  $K_{\mu\mu}^{(n)}(q)$ , where  $\mu = x, y$  and  $n = 0, 1, 3$ . We find that all of them are simply related to their longitudinal counterparts (17)–(19): For  $H_-$  we obtain<sup>20</sup>

$$\begin{aligned} K_{xx}^{(n)}(q) &= [(1-\gamma)/2\gamma] K_z^{(n)}(q), \\ K_{yy}^{(n)}(q) &= [(1+\gamma)/2\gamma] K_z^{(n)}(q), \quad n = 0, 1, 3. \quad (24) \end{aligned}$$

It is therefore tempting to conjecture that the same structural similarity as observed in (24) for the frequency moments also holds for the three components of  $S_{\mu\mu}(q, \omega)$  itself. This conclusion, however, would be in apparent contradiction to rigorous results found by McCoy *et al.*<sup>19</sup>  $S_{xx}(q, \omega)$  and  $S_{yy}(q, \omega)$  of the model (4) at  $h = h_N$  are the subject of planned further investigations.

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<sup>1</sup>A recent comprehensive account of spin-wave theory is found in D. C. Mattis, *Theory of Magnetism I*, Vol. 17 of the *Springer Series in Solid State Sciences* (Springer, Berlin, 1981).

<sup>2</sup>For a recent systematic treatment of linear spin-wave theory for a large class of spin Hamiltonians with extensive references to the earlier literature, see C. A. M. Mulder, H. W. Capel, and J. H. H. Perk, *Physica (Utrecht)* **112B**, 147 (1982).

<sup>3</sup>The original system containing  $N$  spins of magnitude  $s$  has  $(2s+1)^N$  eigenstates. In the LSW approximation, the number of excitations is infinite even for a finite system.

<sup>4</sup>In some cases, depending on the symmetry of  $H$ , the one-magnon states of LSW theory are exact eigenstates of  $H$  itself.

<sup>5</sup>Except for those special cases where LSW theory is exact.

<sup>6</sup>For a recent review of 1D quantum spin dynamics, see H. Beck, M. W. Puga, and G. Müller, *J Appl. Phys.* **52**, 1998 (1981).

<sup>7</sup>P. W. Anderson, *Phys. Rev.* **86**, 694 (1952) has estimated the magnitude of the  $T=0$  sublattice magnetization of the Heisenberg antiferromagnetic  $H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$  for the linear chain ( $D=1$ ), the square lattice ( $D=2$ ), and the simple cubic lattice ( $D=3$ ). His results were the following:  $|\langle \vec{S}_j \rangle| = 0$  for  $D=1$ ,  $|\langle \vec{S}_j \rangle| = S - 0.197$  for  $D=2$ ,  $|\langle \vec{S}_j \rangle| = S - 0.078$  for  $D=3$ .

<sup>8</sup>By fully ordered ground state we mean a state with saturated sublattice magnetizations. The number of sublattices is one

for the ferromagnetic ground state and two for the spin-flop state.

<sup>9</sup>In the classical limit  $s \rightarrow \infty$ , the relative spin deviation  $\Delta S/S$  from the ground-state configuration can be arbitrarily small in an excited state. There exist, therefore, small amplitude excitations (spin waves) for which the anharmonicities in  $H$  are negligible. Hence in the classical limit, LSW theory is exact at  $T=0$ . Under special symmetry conditions such as encountered in Eq. (3) for  $\Delta \geq 1$ , the anharmonicities of  $H$  may have no effect on some excitations (one-magnon states) with the result that LSW theory is exact at  $T=0$  even for finite  $s$ .

<sup>10</sup>C. N. Yang and C. P. Yang, *Phys. Rev.* **147**, 303 (1966); J. Des Clorizeaux and M. Gaudin, *J. Math. Phys.* **7**, 1384 (1966).

<sup>11</sup>E. Lieb, T. Schultz, and D. Mattis, *Ann. Phys. (N.Y.)* **16**, 406 (1961); S. Katsura, *Phys. Rev.* **127**, 1508 (1962); B. M. McCoy, *ibid.* **173**, 531 (1968); E. Barouch and B. M. McCoy, *Phys. Rev. A* **3**, 786 (1971).

<sup>12</sup>J. Kurmann, H. Thomas, and G. Müller, *Physica (Utrecht)* **112A**, 235 (1982).

<sup>13</sup>Such a special value  $h_N$  for the magnetic field where the ground state factorizes into single-site states exists for the more general XYZ antiferromagnet with arbitrary  $s$  and arbitrary field direction  $H = J \sum_{i=1}^N (J_x S_i^x S_{i+1}^x + J_y S_i^y S_{i+1}^y$

$+ J_z S_i^z S_{i+1}^z - \vec{h} \cdot \vec{S}_i)$  (see Ref. 12).

<sup>14</sup>Both  $|G\rangle_+$  and  $|G\rangle_-$  are one component of twofold-degenerate ground states, the other components being obtained by taking the solution  $-\theta$  of Eq. (9b).

<sup>15</sup>T. Niemeijer, *Physica (Utrecht)* **36**, 377 (1967); S. Katsura, T. Horiguchi, and M. Suzuki, *ibid.* **46**, 67 (1976); J. H. H. Perk, H. W. Capel, and T. J. Siskens, *ibid.* **89A**, 304 (1977).

<sup>16</sup>Explicit expressions for  $S_{\alpha\alpha}(q, \omega)$  of (4) with  $s = \frac{1}{2}$  have previously been obtained for the following special cases: (i)  $\gamma=0$ , arbitrary  $h$  by G. Müller, H. Thomas, H. Beck, and J. C. Bonner, *Phys. Rev. B* **24**, 1429 (1981); (ii)  $h=0$ ,  $0 \leq \gamma \leq 1$  by M. W. Puga and H. Beck, *J. Phys. C* **15**, 2441 (1981), M. Mohan and G. Müller, *Phys. Rev. B* **27**, 1776 (1983); (iii)  $\gamma=1$ , arbitrary  $h$  by J. H. Taylor (unpublished).

<sup>17</sup>G. Müller, *Phys. Rev. B* **26**, 1311 (1982).

<sup>18</sup>For the model studied in Ref. 17,  $m$  was fixed:  $m = n + 1$ .

<sup>19</sup>B. M. McCoy, E. Barouch, and D. B. Abraham, *Phys. Rev. A* **4**, 2331 (1971).

<sup>20</sup>The canonical transformation between  $H_+$  and  $H_-$  given in Eqs. (5) and (6) implies that  $S_{\mu\mu}(q, \omega)$ ,  $\mu=x, y$ , of  $H_+$  is equal to  $S_{\mu\mu}(\pi-q, \omega)$  of  $H_-$ . Analogous relations, of course, hold for the quantities  $K_{\mu\mu}^{(n)}(q)$ ,  $\mu=x, y$ .