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Sum rules in the dynamics of quantum spin chains

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An infinite set of sum rules is derived for the dynamics of one-dimensional quantum spin systems. They are employed to derive valuable information on the spectral-weight distribution in the $T=0$ dynamic structure factor $S_{\mu\mu}(q,\omega)$. Applications are presented for various special cases of the nearest-neighbor *XXZ* model, including cases with a discrete excitation spectrum and cases with a continuous spectrum. For the $S=\frac{1}{2}$ *XY*-Heisenberg antiferromagnet, an analytic expression for $S_{zz}(q,\omega)$ is conjectured which satisfies the infinite set of sum rules. In the *XY* limit this expression is identical to the known exact result. A similar conjecture applied to the isotropic Heisenberg antiferromagnet with arbitrary spin quantum number S illustrates how the continuous spectrum of the quantum antiferromagnet collapses into a discrete branch of antiferromagnetic spin waves in the classical limit $S\rightarrow\infty$.

I. INTRODUCTION

Several one-dimensional (1D) spin model systems are exactly solvable at least to some aspects. For their dynamical properties, however, only very few rigorous results are available. The dynamics of the 1D classical Heisenberg (HB) model and related models is highly nontrivial except for $T\rightarrow 0$ where the system goes into a fully ordered state. At $T=0$ linear spin-wave theory is exact. By contrast, the ground state (GS) of quantum spin chains has in general a very complicated structure due to zero-point motion (quantum fluctuations). In some prominent cases it is without true long-range order. Thus, even the $T=0$ dynamics is nontrivial and therefore very interesting.[1]

Several approaches to calculate the excitation spectrum of quantum spin chains have been employed. Those approaches which start from the correct quantum ground state include (i) Bethe ansatz techniques,[2–8] (ii) calculations in the fermion representation,[9–15] and (iii) the mapping between the eight-vertex model and the quantum spin chain.[16] Rigorous results for dynamic correlation functions, however, have essentially been limited to the $S=\frac{1}{2}$ *XY* model.[17] For other models a number of approximate approaches have been used in order to calculate dynamical correlation functions. Valuable results have been obtained by (i) perturbation calculations in the fermion representation,[18–20] (ii) calculations in the continuum approximation (Luttinger model),[21,22] (iii) Holstein-Primakoff-type expansions,[23,24] (iv) perturbation calculations using Ising basis functions,[25] and (v) finite-chain calculations.[6,19,26,27]

In many cases, the results thus obtained are evidently not satisfactory, either because they are contradictory to exact results or they exhibit unphysical features. Moreover, a danger of overinterpretation is inherent in any approximate approach if its accuracy cannot be estimated. Under these circumstances it is important to have a device in hand which can be used to test the validity of dynamical results obtained by approximate techniques. Sum rules are such a device. They have originally been introduced by Hohenberg and Brinkman[28] to 1D quantum spin dynamics, albeit in a very specific and limited form. This paper presents a generalization of the sum rules introduced by Hohenberg and Brinkman to an infinite set, and it describes a novel way to derive information on the $T=0$ dynamics of quantum spin chains from this infinite set of sum rules.

In Sec. II various dynamic quantities are defined and some of their general properties briefly discussed. The infinite set of sum rules is introduced in a general form. In Sec. III A the general properties of these sum rules are derived for the 1D *XXZ* model. Applications to cases with a discrete spectrum [$S=\frac{1}{2}$ HB-Ising ferromagnet (FM), $S\rightarrow\infty$ *XY*-HB antiferromagnet (AFM)] and to a case with a continuous spectrum ($S=\frac{1}{2}$ *XY*-HB AFM) are discussed in Secs. III B and III C, respectively. Section III D deals with the isotropic

HB AFM for $\frac{1}{2} \leq S < \infty$. Here, the sum rules imply that the continuous spectrum collapses into a discrete one in the classical limit $S \to \infty$.

II. FUNDAMENTALS

Dynamical properties of a general many-body system with Hamiltonian H are usually described in terms of a time-dependent correlation function

$$\tilde{S}_{AB}(t) \equiv \langle A(t)B(0)\rangle - \langle A\rangle\langle B\rangle \tag{2.1}$$

for operators A and B, where

$$\langle A\rangle = \mathrm{Tr}[\exp(-\beta H)A] \ ,$$

$\beta = 1/k_B T$, or by its Fourier transform, the dynamic structure factor

$$S_{AB}(\omega) \equiv \int_{-\infty}^{+\infty} dt\, e^{i\omega t}\tilde{S}_{AB}(t) \ . \tag{2.2}$$

A quantity equivalent to (2.1) is the absorptive part of the response function as given by Kubo's formula

$$\tilde{\chi}''_{AB}(t) = \tfrac{1}{2}\langle [A(t),B]\rangle \ . \tag{2.3}$$

Its Fourier transform is related to $S_{AB}(\omega)$ by the fluctuation-dissipation theorem

$$S_{AB}(\omega) = 2\chi''_{AB}(\omega)[1-\exp(-\beta\omega)]^{-1} \ . \tag{2.4}$$

It is useful to recall the properties $\chi''_{AB}(-\omega) = -\chi''_{BA}(\omega)$, $S_{AB}(-\omega) = e^{-\beta\omega}S_{BA}(\omega)$.

The static susceptibility χ_{AB} and the equal-time correlation function Φ_{AB} are obtained from the dynamic quantities $\chi''_{AB}(\omega)$ and $S_{AB}(\omega)$, respectively, through the sum rules

$$\chi_{AB} = 2\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi}\omega^{-1}\chi''_{AB}(\omega) \ , \tag{2.5}$$

$$\Phi_{AB} \equiv \langle AB\rangle - \langle A\rangle\langle B\rangle = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} S_{AB}(\omega) \ . \tag{2.6}$$

Further sum rules for $S_{AB}(\omega)$ or $\chi''_{AB}(\omega)$ are derived from derivatives of $\tilde{\chi}''_{AB}(t)$

$$\frac{d^n}{dt^n}\tilde{\chi}''_{AB}(t) = (-i)^n \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi}\omega^n e^{-i\omega t}\chi''_{AB}(\omega) = \tfrac{1}{2}(-i)^n\langle [[\cdots[[A(t),H],H],\ldots,H],B]\rangle \tag{2.7}$$

taken at $t=0$:

$$K_{AB}^{(n)} = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi}\omega^n \chi''_{AB}(\omega) = \tfrac{1}{2}\langle [[\cdots[[A,H],H],\ldots,H],B]\rangle, \quad n=1,2,3,\ldots \tag{2.8}$$

(where the commutator on the right-hand side is n-fold). The frequency moments $K_{AB}^{(n)}$ are then the coefficients in a Taylor series of $\tilde{\chi}''_{AB}(t)$ around $t=0$. In the important case $A=A^\dagger=B$, both $\tilde{\chi}''_{AA}(t)$ and $\chi''_{AA}(\omega)$ are real odd functions. Here, only the moments with odd n are nonzero in (2.8). At $T=0$ (2.4) (for the case $A=A^\dagger=B$) becomes $S_{AA}(\omega) = 2\chi''_{AA}(\omega)\Theta(\omega)$ where $\Theta(x)$ is the step function. Here (2.5) and (2.8) can also be expressed as frequency moments of $S_{AA}(\omega)$.

$$\chi_{AA} = 2\int_0^\infty \frac{d\omega}{2\pi}\omega^{-1}S_{AA}(\omega), \quad T=0 \tag{2.9}$$

$$K_{AA}^{(n)} = \int_0^\infty \frac{d\omega}{2\pi}\omega^n S_{AA}(\omega) \ , \quad n=1,3,5,\ldots, \ T=0 \ . \tag{2.10}$$

The explicit knowledge of a number of frequency moments $K_{AB}^{(n)}$ can be used for a short-time expansion of $\tilde{\chi}''_{AB}(t)$, or for a continued-fraction representation of the corresponding relaxation function. It is clear, however, that in general these approaches cannot give reliable results for $S_{AB}(\omega)$ unless a great many frequency moments are known. In the following sections the sum rules (2.8) will be employed in a completely different way. It will be demonstrated how information on the structure of $S_{AB}(\omega)$ can be deduced from some general properties of the quantities $K_{AB}^{(n)}$ for the case of 1D spin systems.

III. SUM RULES FOR THE EXCITATION SPECTRUM OF 1D SPIN SYSTEMS

A. General properties

Here we shall investigate some applications of the frequency moments (2.8) for the $T=0$ dynamics of 1D spin systems, in particular the 1D XXZ model. The Hamiltonian reads

$$H = \sum_{l=1}^{N} [J_\perp(S_l^x S_{l+1}^x + S_l^y S_{l+1}^y) + J_z S_l^z S_{l+1}^z] \tag{3.1}$$

with periodic boundary conditions assumed. Depending on the signs and relative size of the coupling strengths $J_\perp$, J_z, the models described by H are known as

(i) HB-Ising FM ($J_z \le J_\perp \le 0$),

(ii) XY-HB FM ($J_\perp \le J_z \le 0$),

(iii) XY-HB AFM ($0 \le J_z \le J_\perp$),

(iv) HB-Ising AFM ($0 \le J_\perp \le J_z$).

The dynamic structure factor for (3.1), as probed by inelastic neutron scattering if H represents a quasi-1D magnet, is given by

$$S_{\mu\mu}(q,\omega)=\sum_R e^{-iqR}\int_{-\infty}^{+\infty} dt\, e^{i\omega t}\langle S_l^\mu(t) S_{l+R}^\mu\rangle, \quad (3.2)$$

$$\mu = x,y,z\ .$$

The symmetry of H requires $S_{xx} \equiv S_{yy}$. At $T=0$ $S_{\mu\mu}(q,\omega)$ can be written as

$$S_{\mu\mu}(q,\omega)=d^{-1}\sum_\lambda M_\lambda^\mu \delta(\omega+E_G-E_\lambda)\ ,$$
$$M_\lambda^\mu=\sum_{i=1}^{d} 2\pi |\langle G_i | S^\mu(q) | \lambda\rangle|^2\ , \quad (3.3)$$

where $|G_i\rangle$, $i=1,\ldots,d$ denotes the d-fold degenerate GS with energy E_G, and the sum λ runs over all eigenstates $|\lambda\rangle$ with energies E_λ. The excitation spectrum of H can be defined as consisting of those excited states which have non-negligible spectral weight M_λ^μ. Depending on the choice of the parameters J_z and $J_\perp$ the excitation spectrum may consist of discrete branches or of continua or of both.[29]

The sum rules (2.8) as applied to the dynamic structure factor $S_{\mu\mu}(q,\omega)$ of the 1D spin system (3.1) at $T=0$ read[30]

$$K_{\mu\mu}^{(n)}(q)\equiv\int_0^\infty \frac{d\omega}{2\pi}\omega^n S_{\mu\mu}(q,\omega)=\tfrac{1}{2}\langle[[\cdots[[S^\mu(q),H],H],\ldots,H],S^\mu(-q)]\rangle,\quad n=1,3,5 \quad (3.4)$$

with

$$S^\mu(q)=N^{-1/2}\sum_{l=1}^{N} e^{iql}S_l^\mu,\quad \mu=x,y,z\ .$$

The explicit evaluation of the multiple commutators in (3.4) is straightforward, but becomes very tedious for $n>1$. The result for $n=1$ reads[28]

$$K_{zz}^{(1)}(q)=-2J_\perp\langle S_l^x S_{l+1}^x\rangle(1-\cos q)\ , \quad (3.5a)$$

$$K_{xx}^{(1)}(q)=-(J_\perp\langle S_l^x S_{l+1}^x\rangle+J_z\langle S_l^z S_{l+1}^z\rangle)+(J_\perp\langle S_l^z S_{l+1}^z\rangle+J_z\langle S_l^x S_{l+1}^x\rangle)\cos q\ . \quad (3.5b)$$

For the Hamiltonian (3.1) the nearest-neighbor correlation functions $\langle S_l^\mu S_{l+1}^\mu\rangle$ can be derived from the GS energy.[27,31] For $S=\frac{1}{2}$, the GS energy is exactly known.[31] Thus, the moments $K_{\mu\mu}^{(1)}(q)$ are fully determined. The result for $K_{zz}^{(3)}(q)$ is relegated to Appendix A. It contains four-point correlation functions which generally are not known, except for special cases where the GS has a simple structure. Evidently, for general n, $K_{\mu\mu}^{(n)}(q)$ is a linear combination of $(n+1)$-point correlation functions with q-dependent coefficients. In Appendix B the important result is proved that $K_{\mu\mu}^{(n)}(q)$, the nth frequency moment of $S_{\mu\mu}(q,\omega)$ for the Hamiltonian (3.1) at $T=0$, is a polynomial in $\cos q$ of degree n:

$$K_{\mu\mu}^{(n)}(q)=\sum_{m=0}^{n} A_m^n \cos^m q\ ,$$
$$A_m^n=\sum_j b_j^{(m)}\langle S_{l_0}^{\beta_0} S_{l_1}^{\beta_1}\cdots S_{l_n}^{\beta_n}\rangle \quad (3.6)$$

with $l_0 \le l_1 \le \cdots \le l_n$, $l_n - l_0 \le n$, $n=1,3,5,\ldots$. This result turns out to be very valuable even without the explicit knowledge of the coefficients A_m^n. Employed as an infinite set of sum rules it can provide important information on the possible structure of $S_{\mu\mu}(q,\omega)$ for the Hamiltonian (3.1) at $T=0$. A few such applications are presented in the following.

B. Discrete spectrum

In cases where the excitation spectrum is known or assumed to consist of a discrete branch $\epsilon_\mu(q)$ and $T=0$ dynamic structure factor has the form

$$S_{\mu\mu}(q,\omega)=2\pi\Phi_{\mu\mu}(q)\delta(\omega-\epsilon_\mu(q))\ , \quad (3.7)$$

where $\Phi_{\mu\mu}(q)$ is the fluctuation intensity (2.6). Here the sum rules (3.6) predict the following general properties of $\epsilon_\mu(q)$ and $\Phi_{\mu\mu}(q)$:

(i) The squared dispersion $\epsilon_\mu^2(q)$ is a quadratic function in $\cos q$:

$$\epsilon_\mu(q)=(C_0+C_1\cos q+C_2\cos^2 q)^{1/2}\ . \quad (3.8)$$

(ii) Two known frequency moments, e.g., $K_{\mu\mu}^{(1)}(q)$ and $K_{\mu\mu}^{(3)}(q)$ are sufficient to fully determine (3.7):

$$\epsilon_\mu(q)=[K^{(3)}_{\mu\mu}(q)/K^{(1)}_{\mu\mu}(q)]^{1/2}\ , \tag{3.9a}$$

$$\Phi_{\mu\mu}(q)=[K^{(1)}_{\mu\mu}(q)]^{3/2}/[K^{(3)}_{\mu\mu}(q)]^{1/2}\ . \tag{3.9b}$$

Further moments are redundant in this case if not useful as a check of consistency for any underlying assumptions. Correspondingly an excitation spectrum consisting of m branches would require at least $2m$ known frequency moments in order to determine the dynamic structure factor.

This case of a discrete spectrum is realized in the $S=\frac{1}{2}$ HB-Ising FM characterized by Hamiltonian (3.1) with $J_z \le J_\perp \le 0$. By rigorous calculations it was shown that the low-lying excitations include a discrete branch of magnon states, a continuum of two-magnon scattering states and an infinite set of magnon bound states.[7,8,16] However, since the GS is well known to be ferromagnetically ordered, it is obvious that only the one-magnon states contribute to $S_{xx}(q,\omega)$ at $T=0$. Since the dispersion of these states

$$\epsilon_M(q)=|J_z|-|J_\perp|\cos q \tag{3.10}$$

is already known, $K^{(1)}_{xx}(q)$ is sufficient to determine $S_{xx}(q,\omega)$, yielding

$$S_{xx}(q,\omega)=\frac{\pi}{2}\delta(\omega-\epsilon_M(q))\ . \tag{3.11}$$

Evidently $\epsilon_M(q)$ has the form (3.8), and (3.11) satisfies the infinite set of sum rules (3.6).

In the case where the Hamiltonian (3.1) has planar anisotropy ($|J_z|\le|J_\perp|$), the GS has no longer a simple structure. For $S=\frac{1}{2}$ it has been shown that, due to strong quantum fluctuations, the correlation functions $\langle S_l^\mu S_{l+R}^\mu\rangle$ decay to zero for large R as a power law.[9,21,32] Accordingly, the excitation spectrum relevant for $S_{\mu\mu}(q,\omega)$ is much more complex (see Sec. III C). It is in the limit $S\to\infty$ only, that the quantum fluctuations become negligible, and the GS is fully ordered. For the planar AFM ($0\le\Delta\le 1$, $\Delta\equiv J_z/J_\perp$, $J_\perp\equiv J$) the classical GS is the familiar Néel state with staggered long-range order in the XY plane, e.g.,

$$\langle S_l^x\rangle=\langle S_l^y\rangle=(-1)^l S/\sqrt{2},\quad \langle S_l^z\rangle=0\ .$$

The further assumption that the excitation spectrum (in the extended Brillouin zone) consists of a single branch of AFM magnons is then consistent with the requirements of the sum rules. The explicity known frequency moments (3.5a) and (A1),

$$K^{(1)}_{zz}(q)=JS^2(1-\cos q)\ , \tag{3.12a}$$

$$K^{(3)}_{zz}(q)=4J^3S^4(1-\cos q)^2(1+\Delta\cos q)\ , \tag{3.12b}$$

determine the out-of-plane component $S_{zz}(q,\omega)$ of the dynamic structure factor according to (3.9) to be

$$S_{zz}(q,\omega)=2\pi\Phi_{zz}(q)\delta(\omega-\epsilon_z(q))\ , \tag{3.13a}$$

$$\epsilon_z(q)=2SJ[(1-\cos q)(1+\Delta\cos q)]^{1/2}\ , \tag{3.13b}$$

$$\Phi_{zz}(q)=\tfrac{1}{2}S[(1-\cos q)/(1+\Delta\cos q)]^{1/2}\ . \tag{3.13c}$$

This is identical to the linear spin-wave result. Evidently (3.13) satisfies the general condition (3.8) and is consistent with the infinite set of sum rules (3.6):

$$K^{(n)}_{zz}(q)=2^{n-1}J^nS^{n+1}(1-\cos q)^{(n+1)/2}\times(1+\Delta\cos q)^{(n-1)/2}=\sum_{m=0}^{n}A^n_m\cos^m q\ . \tag{3.14}$$

In the same way the linear spin-wave result for the in-plane component $S_{xx}(q,\omega)$ can be obtained from sum rules.

Thus, the two assumptions that the classical GS is realized and that the excitation spectrum consists of only one branch have led to a fully consistent picture in the framework of the sum rules (3.6), reproducing the classical spin-wave results. We have to be aware, however, that the sum rules as applied here do not answer the following two questions: (i) Under what circumstances is the classical GS realized in Hamiltonian (3.1)? (ii) Is the assumption of a simple discrete spectrum realistic for the case under investigation? An example of a system with a classical (two-sublattice) GS but a rather complex excitation spectrum is realized in the anisotropic XYZ AFM in a magnetic field.[33,34]

C. Continuous spectrum

In the case where the excitation spectrum of the Hamiltonian (3.1) consists of one or several continua, there has been no direct, practical way of deducing the detailed structure of $S_{\mu\mu}(q,\omega)$ from any finite number of frequency moments.[35] Previous dynamical investigations employing sum rules have therefore been limited to qualitative considerations. Calculations for the quantum chain[28,36] have relied on $K^{(1)}_{\mu\mu}(q)$ only.[37] Also in calculations for the classical chain (in the form of a continued-fraction expansion) the number of sum rules used has been rather small.[38,39] It is the availability of the infinite set of sum rules (3.6) which allows us to make more precise statements on the structure of $S_{\mu\mu}(q,\omega)$.

In this section we shall concentrate on the $S=\frac{1}{2}$ XY-HB AFM, i.e., (3.1) with $(0\le\Delta\le 1,\ \Delta\equiv J_z/J_\perp,\ J_\perp\equiv J)$, as an example of a system with a continuous excitation spectrum. In previous work[6,27] it has been demonstrated that $S_{zz}(q,\omega)$ at $T=0$ is dominated by a two-parameter continuum of excitations with energies

$$\epsilon(k,q)=J(\pi\sin\mu/\mu)\sin\frac{q}{2}\cos\left[\frac{q}{2}-\frac{k}{2}\right],\tag{3.15}$$

$$\Delta=\cos\mu,\quad 0\le k\le q\le\pi\ .$$

The continuum is bounded by the two branches

$$\begin{aligned}\epsilon_L(q)&=J(\pi\sin\mu/2\mu)\sin q\ ,\\ \epsilon_U(q)&=(\pi\sin\mu/\mu)\sin\frac{q}{2}\ .\end{aligned}\tag{3.16}$$

The exact $S_{zz}(q,\omega)$ is known only for the XY model $(\Delta=0)$ (Refs. 10 and 11):

$$S_{zz}(q,\omega)=2\frac{\Theta(\omega-\epsilon_L(q))\Theta(\epsilon_U(q)-\omega)}{[\epsilon_U^2(q)-\omega^2]^{1/2}}\ .\tag{3.17}$$

This result reflects the density of states in the continuum (3.15). For $\Delta=0$ the matrix elements M_λ^z of (3.3) are nonzero and constant for the states (3.15) and zero for all the other states. It has been shown by finite-chain calculations that for (3.1) with $0<\Delta\le 1$ the continuum states (3.15) still predominate $S_{zz}(q,\omega)$, but the matrix elements are no longer constant.[6,27] Approximate calculations based on two different approaches[20–22] have consistently led to the conclusion that this discontinuity in $S_{zz}(q,\omega)$ at $\omega=\epsilon_L(q)$ present for $\Delta=0$ changes to a power-law singularity of the form $[\omega^2-\epsilon_L^2(1)]^{-\alpha}$ for nonzero Δ. On the other hand, extrapolations of finite-chain calculations suggest that the matrix elements (more precisely, the quantities NM_λ^z) of the continuum states go continuously to zero if their energies approach the upper bound $\epsilon_U(q)$.[40] This indicates that the divergence in $S_{zz}(q,\omega)$ at $\omega=\epsilon_U(q)$, which is due to a divergent density of states, becomes weaker for $\Delta>0$ than in (3.17) for $\Delta=0$.

All this suggests a conjecture for the continuum contribution to $S_{zz}(q,\omega)$ of the general form

$$S_{zz}(q,\omega)=\text{const}\times[\omega^2-\epsilon_L^2(q)]^{-\alpha}[\epsilon_U^2(q)-\omega^2]^{-\beta}\ ,\tag{3.18}$$

$$\epsilon_L(q)\le\omega\le\epsilon_U(q)\ .$$

It is the simplest generalization of the XY result (3.17) which is compatible with the above-mentioned results from approximate approaches and finite-chain calculations.[41]

The validity of (3.18) will now be checked by the severe test of the infinite set of sum rules (3.6). The nth frequency moment of (3.18) can be evaluated exactly yielding[42]

$$K_{zz}^{(n)}(q)=\text{const}\times(u^2)^{(n-1)/2+2(1-\alpha-\beta)}(1-u^2)^{(n-1)/2}\,{}_2F_1\left[-\frac{n-1}{2},1-\alpha;2-\alpha-\beta;\frac{u^2}{1-u^2}\right]\tag{3.19}$$

with $u=\sin(q/2)$, $n=1,3,5.\ldots$ The hypergeometric function ${}_2F_1$ for negative integer first arguments $-(n-1)/2$ can be written as polynomial[43]

$${}_2F_1\left[-\frac{n-1}{2},1-\alpha;2-\alpha-\beta;\frac{u^2}{1-u^2}\right]=\sum_{l=0}^{\frac{n-1}{2}}\frac{\left[\frac{n-1}{2}\right]_l(1-\alpha)_l}{(2-\alpha-\beta)_l\,l!}\left[\frac{u^2}{1-u^2}\right]^l,\tag{3.20}$$

where $(a)_l=\Gamma(a+l)/\Gamma(a)$ is Pochhammer's symbol. We notice at once that (3.19) with (3.20) reduces to a polynomial in $\cos q$ of degree n exactly if the two exponents α,β are related to each other by $\alpha+\beta=\frac{1}{2}$. Hence, the infinite set of sum rules (3.6) is in strong support of the following conjecture for $S_{zz}(q,\omega)$ of the $S=\frac{1}{2}$ XY-HB AFM at $T=0$:

$$S_{zz}(q,\omega)=\frac{2A}{B(1-\alpha,\frac{1}{2}+\alpha)}\frac{\Theta(\omega-\epsilon_L(q))\Theta(\epsilon_U(q)-\omega)}{[\omega^2-\epsilon_L^2(q)]^{\alpha}[\epsilon_U^2(q)-\omega^2]^{1/2-\alpha}}\tag{3.21}$$

with the beta function as a convenient normalizing factor. The rigorous XY result (3.17) is recovered with $\alpha=0, A=2$. The frequency moments then read (with $p=J\pi\sin\mu/\mu$)

$$K_{zz}^{(n)}(q)=\frac{Ap^n}{2\pi}\sum_{l=0}^{\frac{n-1}{2}}\frac{\left[-\frac{n-1}{2}\right]_l (1-\alpha)_l}{(\frac{3}{2})_l l!}(u^2)^{(n+1)/2+l}(1-u^2)^{(n-1)/2-l}=\sum_{m=0}^{n}A_m^n\cos^m q,\quad n=1,3,5.\ldots \tag{3.22}$$

The normalization constant A is determined by $K_{zz}^{(1)}(q)$ of (3.5a), the only frequency moment which is completely known. The determination of the exponent α in (3.21) would require the *complete* knowledge of one further frequency moment, e.g., $K_{zz}^{(3)}(q)$, i.e., expression (A1) including the values of the four-point correlation functions. As these higher correlation functions are not known for the $S=\frac{1}{2}$ planar AFM, a different way for determining α has to be found. Luther and Peschel,[21] by using the mapping between the quantum spin chain and the eight-vertex model, have related $T=0$ critical exponents of the $S=\frac{1}{2}$ planar AFM to known critical exponents of the eight-vertex model. Their results imply a Δ-dependent exponent α

$$\alpha=(\pi/2-\mu)/(\pi-\mu),\quad \cos\mu=\Delta\ . \tag{3.23}$$

To $O(\Delta)$ this exponent is reproduced by approximate calculations in the fermion representation of (3.1): (i) by calculations in the continuum limit (Luttinger model)[21,22] yielding results valid for $\omega \ll J$ (i.e., $q\simeq 0$ and $q\simeq\pi$), and (ii) by dynamical Hartree-Fock calculations for the lattice spin model,[20] yielding results which are valid for all wave numbers.

Note that the expression (3.21) has already been conjectured in a previous pubication.[27] However, it is only now that its validity is supported by an infinite set of sum rules. The implications of the result (3.21) for various physical quantities of interest including the determination of the constant A are extensively discussed in Ref. 27. Here the result (3.21) for $S_{zz}(q,\omega)$ shall be compared with the same quantity as obtained by a perturbation calculation in the fermion representation. In this approach which does not make use of sum rules the XY part of the Hamiltonian (3.1) represents a system of free fermions and the part multiplied by J_z an interaction between the fermions. $S_{zz}(q,\omega)$ is related to a two-particle Green's function. This has been calculated for the planar AFM in the Hartree-Fock approximation.[18,20] At $\Delta=0$ both approaches yield the exact result (3.17), which has a finite step at $\epsilon_L(q)$ and a square-root divergence at $\epsilon_U(q)$. At $\Delta=0.1$, the result (3.21) [for $q=4\pi/5$ shown as a solid line in Fig. 1(a)] has developed a second power-law divergence at $\epsilon_L(q)$ where the step discontinuity was, and the singularity at $\epsilon_U(q)$ has become weaker. The dashed line in Fig. 1(a) represents the corresponding Hartree-Fock result[44] for the line shape of $S_{zz}(4\pi/5,\omega)$. $\Delta=0.1$ belongs to the weak-coupling regime in the fermion representation. Therefore, we can expect the Hartree-Fock approximation to reproduce a qualitatively correct picture. $S_{zz}(q,\omega)$ indeed has also the characteristic two-peak structure. Evidently, the fact that the two peaks are rounded off (one of them being very sharp and tall) is an artifact of the Hartree-Fock approximation. A more careful

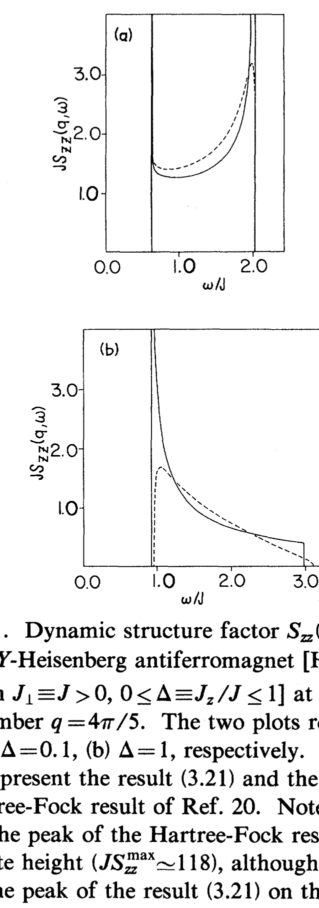

FIG. 1. Dynamic structure factor $S_{zz}(q,\omega)$ for the $S=\frac{1}{2}$ XY-Heisenberg antiferromagnet [Hamiltonian (3.1) with $J_\perp\equiv J>0$, $0\leq\Delta\equiv J_z/J\leq 1$] at $T=0$ and fixed wave number $q=4\pi/5$. The two plots represent the cases (a) $\Delta=0.1$, (b) $\Delta=1$, respectively. The solid curves represent the result (3.21) and the dashed curves the Hartree-Fock result of Ref. 20. Note that for $\Delta=0.1$ the peak of the Hartree-Fock result at $\omega\simeq\epsilon_L(q)$ is of finite height ($JS_{zz}^{\max}\simeq 118$), although very sharp and high. The peak of the result (3.21) on the other hand, is of infinite height.

analysis reveals, however, that a power-law singularity of the form $[\omega^2-\epsilon_L^2(q)]^{-\alpha}$ appears in the Hartree-Fock result as a logarithmic correction.[20] For $\Delta=1$, the result (3.21) has a square-root divergence at $\epsilon_L(q)$ and a finite step at $\epsilon_U(q)$. The line shape of $S_{zz}(4\pi/5,\omega)$ is shown as a solid line in Fig. 1(b). $\Delta=1$ is no longer in the weak-coupling regime. Therefore, we cannot expect a reliable result from the Hartree-Fock calculation [see dashed line in Fig. 1(b)]. It displays indeed a much less pronounced peak close to $\epsilon_L(q)$.

D. Transition from continuous to discrete spectrum

We note that the general properties of the sum rules (3.4) satisfied by (3.21) are independent of the spin quantum number S. This indicates that the validity of (3.21) is not necessarily restricted to $S=\frac{1}{2}$ chains. In a previous publication,[27] arguments were indeed presented which suggest that $S_{zz}(q,\omega)$ for the isotropic $S\geq\frac{1}{2}$ HB AFM [i.e., (3.1) with $J_z=J_\perp\equiv J>0$] can still be represented by an expression of the form (3.21) with continuum boundaries $\epsilon_L(q)=(p/2)\sin q$, $\epsilon_U(q)=p\sin(q/2)$. In the quantum limit $S=\frac{1}{2}$, $S_{zz}(q,\omega)$ is characterized by the parameters $p=\pi J$, $\alpha=\frac{1}{2}$, $A=\frac{8}{3}(\ln 2-\frac{1}{4})$, according to the results of Sec. III C.[45] Now we use the sum rules for the determination of the same parameters in the classical limit $S\rightarrow\infty$. For the classical GS $\langle S_l^x\rangle=\langle S_l^y\rangle=\langle S_l^z\rangle=(-1)^l S/\sqrt{3}$, the correlation function in the sum rules (3.5a) and (4.1) can be evaluated explicitly, yielding

$$K_{zz}^{(1)}(q)=\tfrac{2}{3}JS^2(1-\cos q)\ , \tag{3.24a}$$

$$K_{zz}^{(3)}(q)=\tfrac{8}{3}J^3S^4(1-\cos q)^2(1+\cos q)\ . \tag{3.24b}$$

The corresponding frequency moments of (3.21) as given by (3.22) are

$$K_{zz}^{(1)}(q)=(AJS/\pi)(1-\cos q)\ , \tag{3.25a}$$

$$K_{zz}^{(3)}(q)=(4AJ^3S^3/\pi)[(1-\cos q)^2(1+\cos q)+\tfrac{2}{3}(1-\alpha)(1-\cos q)^3]\ , \tag{3.25b}$$

where the amplitude predicted by classical spin-wave theory $p=2JS$ has been used.

Comparison of (3.24) and (3.25) demonstrates that with

$$\alpha=1,\quad A=2\pi S/3\ , \tag{3.26}$$

the conjecture (3.21) is adequate for the HB AFM in the classical limit. It is readily proved that for this set of parameters expression (3.21) is equivalent to the prediction of linear spin-wave theory

$$S_{zz}(q,\omega)=\tfrac{2}{3}\pi S[(1-\cos q)/(1+\cos q)]^{1/2}\times\delta(\omega-2JS\sin q)\ . \tag{3.27}$$

In the limit $\alpha\rightarrow 1$ the divergence of (3.21) at $\epsilon_L(q)=2JS\sin q$ becomes very strong; simultaneously the normalizing factor $2A/B(1-\alpha,\frac{1}{2}+\alpha)$ tends to zero, leaving nonzero intensity only at $\omega=\epsilon_L(q)$. Thus the sum rules force the continuous spectrum of the 1D quantum HB AFM to collapse into a discrete spectrum as the classical limit is approached.

The conjecture (3.21) in combination with the sum rules offers a practical way to obtain quantum corrections to the classical result (3.27) by calculating quantum corrections to the static correlation functions appearing in $K_{zz}^{(1)}(q)$ and $K_{zz}^{(3)}(q)$. A rough estimate of such quantum corrections can be done by approximating the four-point correlation functions of (A1) as products of pair correlation functions $\langle S_l^\mu S_{l+R}^\mu\rangle$, $R=0,1$.

With

$$|\langle S_l^x S_{l+R}^x\rangle|=|\langle S_l^y S_{l+R}^y\rangle|=|\langle S_l^z S_{l+R}^z\rangle|\equiv F_R\ ,$$

$R=0,1$, the sum rules (3.5a) and (A1) then read

$$K_{zz}^{(1)}(q)=2JF_1(1-\cos q)\ , \tag{3.28a}$$

$$K_{zz}^{(3)}(q)=24J^3F_1[(F_1+F_0)(1-\cos q)^2-F_1(1-\cos q)^3]\ . \tag{3.28b}$$

By comparing (3.28) and (3.25), the quantum corrections in the parameters A,α of expression (3.21) for $S_{zz}(q,\omega)$ are determined in terms of quantum corrections to F_1. For the exponent α we thus get

$$\alpha=3F_1/(F_1+F_0)-\tfrac{1}{2}\ . \tag{3.29}$$

Using the results $F_0=\frac{1}{3}S^2$, $F_1=\frac{1}{3}S^2(1-2/\pi S)$ of linear spin-wave theory,[46] (3.29) yields to $O(S^{-1})$

$$\alpha=1-\frac{3}{2\pi S}\ . \tag{3.30}$$

This has to be compared with a result by Mikeska.[23] He calculated quantum corrections to $S_{zz}(q,\omega)$ of the HB AFM at $T=0$ by use of a Holstein-Primakoff-type approach (boson representation), and found an analytic result for

$q \simeq \pi$, $\omega \ll 2JS$:

$$S_{zz}(q,\omega) \propto \Theta(\omega - 2JS\sin q) \times (\omega^2 - 4J^2S^2\sin^2 q)^{-\alpha'}$$

with an exponent $\alpha' = 1 - 1/\pi S + O(S^{-2})$ very similar to (3.30). In view of the crude approximations used for the four-point correlation functions in (3.28b), the agreement is reasonable.

In summary, some general properties of an infinite set of sum rules for the dynamics of 1D quantum spin chains have been derived and their implications on the properties of the $T=0$ dynamic structure factor $S_{\mu\mu}(q,\omega)$ discussed for various cases in the general *XXZ* model. In cases with a discrete spectrum, $S_{\mu\mu}(q,\omega)$ is directly determined from known sum rules. For the $S=\frac{1}{2}$ *XY*-HB AFM and for the isotropic $S > \frac{1}{2}$ HB AFM, i.e., cases with a continuous spectrum, an analytic expression for $S_{zz}(q,\omega)$ at $T=0$ has been conjectured which satisfies all the sum rules. For the latter model it is shown how the continuous spectrum transforms into a discrete one in the classical limit $S \to \infty$.

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APPENDIX A: EXACT RESULT FOR $K_{zz}^{(3)}(q)$

The sum rule $K_{zz}^{(3)}(q)$ determining the third frequency moment of the dynamic structure factor $S_{zz}(q,\omega)$ for the Hamiltonian (3.1) has been calculated in terms of four-point correlation functions. The result reads ($J_\perp \equiv J$, $\Delta = J_z/J$):

$$\begin{aligned}
K_{zz}^{(3)}(q) &= 4J^3 \left[\sum_{m=1}^{4} Q_m(q) + \Delta \sum_{m=5}^{9} Q_m(q) + \Delta^2 Q_{10}(q) \right], \\
Q_1(q) &= -2\langle S_l^x S_{l+1}^z S_{l+2}^z S_{l+3}^x \rangle (1-\cos q)^3, \\
Q_2(q) &= \{ 3\langle S_l^x S_{l+1}^z S_{l+2}^z S_{l+3}^x \rangle - \langle S_l^x S_{l+1}^x S_{l+2}^x S_{l+2}^x \rangle \\
&\quad - \langle S_l^x S_{l+1}^y S_{l+2}^y S_{l+2}^x \rangle - \langle S_l^x S_{l+1}^z S_{l+1}^x S_{l+2}^z \rangle \} (1-\cos q)^2, \\
Q_3(q) &= \{ \langle S_l^x S_l^x S_{l+1}^x S_{l+2}^x \rangle + \langle S_l^x S_l^x S_{l+1}^y S_{l+2}^y \rangle \\
&\quad + \langle S_l^x S_{l+1}^x S_{l+1}^z S_{l+2}^z \rangle + \langle S_l^x S_{l+1}^z S_{l+1}^x S_{l+2}^z \rangle \} \cos q (1-\cos q), \\
Q_4(q) &= -\{ \langle S_l^x S_l^x S_l^x S_{l+1}^x \rangle + \langle S_l^x S_l^x S_l^y S_{l+1}^y \rangle + \langle S_l^x S_l^z S_{l+1}^x S_{l+1}^z \rangle + \langle S_l^x S_l^z S_{l+1}^z S_{l+1}^x \rangle \} (1-\cos q), \\
Q_5(q) &= -2\{ \langle S_l^x S_{l+1}^x S_{l+2}^x S_{l+3}^x \rangle + \langle S_l^x S_{l+1}^x S_{l+2}^y S_{l+3}^y \rangle \} (1-\cos q)^3, \\
Q_6(q) &= \{ 4\langle S_l^x S_{l+1}^x S_{l+2}^x S_{l+3}^x \rangle + 4\langle S_l^x S_{l+1}^x S_{l+2}^y S_{l+3}^y \rangle - \langle S_l^x S_{l+1}^y S_{l+2}^y S_{l+3}^x \rangle \\
&\quad + \langle S_l^x S_{l+1}^y S_{l+2}^x S_{l+3}^y \rangle - \langle S_l^x S_{l+1}^x S_{l+1}^y S_{l+2}^y \rangle - \langle S_l^x S_{l+1}^y S_{l+1}^x S_{l+2}^y \rangle \} (1-\cos q)^2, \\
Q_7(q) &= 2\langle S_l^x S_{l+1}^x S_{l+1}^x S_{l+2}^x \rangle \cos q (1-\cos q), \\
Q_8(q) &= \{ \langle S_l^z S_l^x S_{l+1}^z S_{l+2}^x \rangle + \langle S_l^x S_l^z S_{l+1}^z S_{l+2}^x \rangle \\
&\quad - \langle S_l^x S_{l+1}^z S_{l+1}^z S_{l+2}^x \rangle - \langle S_l^z S_{l+1}^x S_{l+2}^z S_{l+3}^x \rangle \} (1-\cos q)(1+\cos q), \\
Q_9(q) &= \{ 2\langle S_l^x S_{l+1}^y S_{l+1}^y S_{l+2}^x \rangle - \langle S_l^x S_{l+1}^x S_{l+2}^x S_{l+3}^x \rangle - \langle S_l^x S_{l+1}^x S_{l+2}^y S_{l+3}^y \rangle - \langle S_l^x S_l^x S_{l+1}^x S_{l+1}^x \rangle \\
&\quad + \langle S_l^x S_l^x S_{l+1}^y S_{l+1}^y \rangle - \langle S_l^x S_l^y S_{l+1}^x S_{l+1}^y \rangle - \langle S_l^x S_l^y S_{l+1}^y S_{l+1}^x \rangle \} (1-\cos q), \\
Q_{10}(q) &= \{ 2\langle S_l^z S_{l+1}^x S_{l+1}^z S_{l+2}^x \rangle + \langle S_l^z S_{l+1}^x S_{l+2}^x S_{l+3}^z \rangle + \langle S_l^x S_l^z S_{l+1}^z S_{l+1}^x \rangle \\
&\quad - 2\langle S_l^z S_{l+1}^x S_{l+2}^z S_{l+2}^x \rangle - \langle S_l^z S_l^z S_{l+1}^x S_{l+2}^x \rangle - \langle S_l^x S_l^z S_l^z S_{l+1}^x \rangle \} (1-\cos q).
\end{aligned} \tag{A1}$$

APPENDIX B: GENERAL PROPERTIES OF $K_{\mu\nu}^{(n)}(q)$

Here some general properties are derived for the quantity (where the commutator on the right-hand side is n-fold)

$$K_{\mu\nu}^{(n)}(q)=\tfrac{1}{2}\langle[[\cdots[[S^{\mu}(q),H],H],\ldots,H],S^{\nu}(-q)]\rangle,\quad n=1,3,5,\ldots,\quad \mu,\nu=x,y,z \tag{B1}$$

of the general XYZ Hamiltonian

$$H=\sum_{l=1}^{N}\{J_xS_l^xS_{l+1}^x+J_yS_l^yS_{l+1}^y+J_zS_l^zS_{l+1}^z\}=\sum_{\mu}J_{\mu}H_{\mu}\ . \tag{B2}$$

(B1) can be decomposed into a sum

$$\begin{aligned}K_{\mu\nu}^{(n)}(q)&=\tfrac{1}{2}\sum_{i=1}^{3^n}a_i\langle k_i(q)\rangle,\quad a_i=J_{\alpha_1}J_{\alpha_2}\cdots J_{\alpha_n}\\ k_i(q)&=[[\cdots[[S^{\mu}(q),H_{\alpha_1}],H_{\alpha_2}],\ldots,H_{\alpha_n}],S^{\nu}(-q)]\\ &=N^{-1}\sum_{ll'}e^{iq(l-l')}[[\cdots[[S_l^{\mu},H_{\alpha_1}],H_{\alpha_2}],\ldots,H_{\alpha_n}],S_{l'}^{\nu}]\ ,\end{aligned} \tag{B3}$$

where i is a short notation for $\{\alpha_1,\alpha_2,\ldots,\alpha_n\}$. To keep the notation simple, the fixed labels μ,ν,n are suppressed in most of the following quantities. The multiple commutator in (B3) has the following general form

$$[[\cdots[[S_l^{\mu},H_{\alpha_1}],H_{\alpha_2}],\ldots,H_{\alpha_n}],S_{l'}^{\nu}]=(i)^{n+1}\sum_j e_j\{f_j\delta_{l'-l,R_j}+\bar{f}_j\delta_{l-l',R_j}\}\ , \tag{B4}$$

where

$$f_j=S_{l_0}^{\beta_0}S_{l_1}^{\beta_1}\cdots S_{l_n}^{\beta_n},\quad \bar{f}_j=S_{\bar{l}_0}^{\beta_0}S_{\bar{l}_1}^{\beta_1}\cdots S_{\bar{l}_n}^{\beta_n},$$

$$l_i=l+R_i,\ \bar{l}_i=l-R_i,\ l_0\le l_1\le\cdots\le l_n,$$

the index j stands for the whole set $\{l_0,\beta_0;l_1,\beta_1;\ldots;l_n,\beta_n\}$, and $e_j=0,\pm1$. Owing to the fact that H is a nearest-neighbor interaction the magnitude of R_j is restricted to $|R_j|<n$. Moreover, the inversion symmetry of H implies $\langle\bar{f}_j\rangle=\langle f_j\rangle$. We thus obtain

$$k_i(q)=(i)^{n+1}\sum_j e_j\langle f_j\rangle\cos(qR_j)\ ,\ |R_j|\le n\ . \tag{B5}$$

Expressing $\cos(qR_j)$ as a polynomial in $\cos q$ of degree n yields the following general form for $K_{\mu\nu}^{(n)}(q)$

$$\begin{aligned}K_{\mu\nu}^{(n)}(q)&=\sum_{m=0}^{n}A_m^n\cos^m q\ ,\\ A_m^n&=\sum_j b_j^{(m)}\langle S_{l_0}^{\beta_0}S_{l_1}^{\beta_1}\cdots S_{l_n}^{\beta_n}\rangle\end{aligned} \tag{B6}$$

where $l_0\le l_1\le\cdots\le l_n$, $l_n-l_0\le n$, $n=1,3,5,\ldots$, and where $b_j^{(m)}$ is an integer.

[1]For recent reviews on the dynamics of classical and quantum spin chains see H. Beck, M. W. Puga, and G. Müller, J. Appl. Phys. 52, 1998 (1981), and the articles by J. C. Bonner, H. W. J. Blöte, H. Beck, and G. Müller, in *Physics in One Dimension*, edited by J. Bernasconi and T. Schneider (Springer, Heidelberg, 1981), p. 115; S. W. Lovesey, *ibid.*, p. 129; M. Steiner, *ibid.*, p. 140.

[2]J. Des Cloizeaux and J. J. Pearson, Phys. Rev. 128, 2131 (1962).

[3]J. Des Cloizeaux and M. Gaudin, J. Math. Phys. 7, 1384 (1966).

[4]J. D. Johnson and B. M. McCoy, Phys. Rev. A 6, 1613 (1972).

[5]N. Ishimura and H. Shiba, Prog. Theor. Phys. 57, 1862 (1977).

[6]G. Müller, H. Thomas, H. Beck, and J. C. Bonner, Phys. Rev. B 24, 1429 (1981).

[7]R. Orbach, Phys. Rev. 112, 309 (1958).

[8]J. D. Johnson and J. C. Bonner, Phys. Rev. B 22, 251

(1980).
[9]E. H. Lieb, T. D. Schultz, and D. C. Mattis, Ann. Phys. (N.Y.) 16, 407 (1961).
[10]T. Niemeijer, Physica 36, 377 (1967).
[11]S. Katsura, T. Horiguchi, and M. Suzuki, Physica 46, 67 (1970).
[12]B. M. McCoy, E. Barouch, and D. B. Abraham, Phys. Rev. A 4, 2331 (1971).
[13]J. H. H. Perk, H. W. Capel, and T. J. Siskens, Physica 89A, 304 (1977).
[14]M. W. Puga and H. Beck, J. Phys. C 15, 2441 (1982).
[15]H. G. Vaidya and C. A. Tracy, Physica 92A, 1 (1978).
[16]J. D. Johnson, S. Krinsky, and B. M. McCoy, Phys. Rev. A 8, 2526 (1973).
[17]Apart from the trivial case of the HB-Ising ferromagnet at $T=0$.
[18]T. Todani and K. Kawasaki, Prog. Theor. Phys. 50, 1216 (1973).
[19]T. Schneider and E. Stoll, J. Appl. Phys. 53, 1850 (1982).
[20]H. Beck and G. Müller, Solid State Commun. (in press).
[21]A. Luther and I. Peschel, Phys. Rev. B 12, 3908 (1975).
[22]H. C. Fogedby, J. Phys. C 11, 4767 (1978).
[23]H. J. Mikeska, Phys. Rev. B 12, 2794 (1975).
[24]G. Reiter (private communications).
[25]N. Ishimura and H. Shiba, Prog. Theor. Phys. 63, 743 (1980).
[26]G. Müller and H. Beck, J. Phys. C 11, 483 (1978).
[27]G. Müller, H. Thomas, M. W. Puga, and H. Beck, J. Phys. C 14, 3399 (1981).
[28]P. C. Hohenberg and W. F. Brinkman, Phys. Rev. B 10, 128 (1974).
[29]The distinction between "discrete" and "continuous" spectrum as used in this paper refers to the spectrum for fixed wave number.
[30]Equations (2.9) and (2.10) are also satisfied for $S_{AB}(\omega)$ with $A=S^{\mu}(q)$, $B=S^{\mu}(-q)$ owing to the reflection symmetry of H.
[31]C. N. Yang and C. P. Yang, Phys. Rev. 150, 327 (1966).
[32]B. M. McCoy, Phys. Rev. 173, 531 (1968).
[33]J. Kurmann, H. Thomas, and G. Müller, Physica A (in press).
[34]J. Kurmann (unpublished).
[35]A remarkable exception was the prediction by A. Sur, D. Jasnow, and I. J. Lowe, Phys. Rev. B 12, 3845 (1975) of the exact $S_{xx}(q,\omega)$ for the $S=\frac{1}{2}$ XY model ($J_z=0$) at $T=\infty$, based on the numerical calculation of 16 frequency moments for finite chains with up to nine spins.
[36]M. Fowler and M. W. Puga, Phys. Rev. B 19, 5906 (1979).
[37]In combination with the additional sum rules (2.6) and (2.9) for $S_{\mu\mu}(q,\omega)$ $q\rightarrow 0$.
[38]S. W. Lovesey, J. Phys. C 7, 2008 (1974).
[39]H. DeRaedt and B. DeRaedt, Phys. Rev. B 15, 5379 (1977).
[40]G. Müller (unpublished).
[41]In Ref. 6 it was shown for $\Delta=1$ that a quantitative analysis of finite-chain matrix elements M_{λ}^{z} is in strong support of such a conjecture (see Fig. 4 of Ref. 6).
[42]I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series, and Products* (Academic, New York, 1965).
[43]M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1972).
[44]The explicit Hartree-Fock result of $S_{zz}(q,\omega)$ is found as Eq. (16) in Ref. 20.
[45]A has been determined in Ref. 27.
[46]P. W. Anderson, Phys. Rev. 86, 694 (1952).