Line shapes of dynamical correlation functions in Heisenberg chains

Ralph Werner
Physics Department, Brookhaven National Laboratory, Upton, NY 11973-5000, USA

Andreas Klümper
Physics Department, University of Dortmund, D-44221 Dortmund, Germany
(March 22, 2022)

Preprint. Typeset using REVTeX

We calculate line shapes of correlation functions by use of complete diagonalization data of finite chains and analytical implications from conformal field theory, density of states, and Bethe ansatz. The numerical data have different finite size accuracy in case of the imaginary and real parts in the frequency and time representations of spin-correlation functions, respectively. The low temperature, conformally invariant regime crosses over at $T_c$ to a diffusive regime that in turn connects continuously to the high temperature, interacting fermion regime. The first moment sum rule is determined.

I. INTRODUCTION

Dynamical correlations characterize the spectral properties of physical systems. They are accessible by a multitude of experimental setups. The access to dynamical correlation functions for physically relevant systems is usually difficult even in exactly solvable models. Dynamical spin-correlation functions in Heisenberg chains have been widely studied numerically as well as analytically. The comparison of numerical and approximate analytical results for the purpose of accuracy control has been used in various previous approaches.

Usually the focus lies on the imaginary part of the correlation functions. The real and the imaginary parts can be Kramers-Kronig transformed into each other and thus hold the same information. This is also true for the Fourier transform. The information that can be extracted from finite systems accessible by exact diagonalization (ED) concerning the thermodynamic limit is limited. The accuracy of the results is different for different representations. In the case of finite systems it proves thus useful to actually calculate all three representations to extrapolate to the thermodynamic limit.

The dynamical correlation functions become system size independent for high excitation energies or, equivalently, on short time scales. While finite systems thus allow for the determination of correlation functions in the thermodynamic limit at high frequencies or on short time scales, field theoretical results describe their asymptotic behavior on long time scales or for small frequencies. The perspective of this paper is to combine the strongholds of both methods.

The system to be discussed here is the one-dimensional antiferromagnetic Heisenberg model

$$H = \sum_{l} \left( J S^x_l S^x_{l+1} + J S^y_l S^y_{l+1} + J_z S^z_l S^z_{l+1} \right)$$

$$+ J_2 \sum_{l} \left( S^z_l S^z_{l+2} + S^y_l S^y_{l+2} + S^z_l S^z_{l+2} \right)$$ (1)

with the superexchange integrals $J$ and $J_2$ between nearest-neighbor (NN) and next-nearest-neighbor (NNN) magnetic ions, respectively, $z$-axis anisotropy $J_z$ and spin-1/2 operator components $S^\nu_l$ with $\nu = x, y, z$ at site $l$. Energies will be given in units of the in plane exchange, i.e., $J \equiv 1$. This Hamiltonian is relevant for the description of the magnetic systems in many quasi-one-dimensional materials as Sr$_2$CuO$_2$Cl$_2$, Cs$_2$CuCl$_4$, KCuF$_3$, or CuGeO$_2$.

We focus on the spin-correlation function

$$\chi(q, i\omega_n) = \frac{1}{L} \int_{0}^{\beta} d\tau \ e^{i\omega_n \tau} \langle S^z_q(\tau) S^z_{-q}(0) \rangle$$ (2)

with Matsubara frequencies $\omega_n = 2\pi n/\beta$, inverse temperature $\beta = 1/T$, ($k_B = 1$) Fourier transformed spin operators in interaction representation $S^\tau_q(\tau) = e^{-iH\tau} \sum_l e^{-iql} S^\nu_l e^{iH\tau}$, and number of sites $L$. In its analytically continued form, where $i\omega_n \to \omega + i\epsilon$ with $\epsilon \to 0$, it determines the structure factor

$$S(q, \omega) = \frac{1}{\pi} \frac{\text{Im} \chi(q, \omega)}{1 - e^{-\beta \omega}}$$ (3)

relevant for neutron scattering experiments.

A. Numerical methods

For finite systems the correlation function can be calculated through the diagonalization of the spin Hamiltonian in the spectral representation since eigenfunctions $|n\rangle$ and eigenvalues $E_n$ are known. All numerical results in this paper are obtained using periodic boundary conditions. Defining the matrix elements

$$V_{nm} = \langle n \mid S^z_q \mid m \rangle$$ (4)

and the Boltzmann factor

$$\frac{1}{\cosh(\beta E_n/2)}$$
where \( Z = \text{Tr} \ e^{-\beta H} \) is the partition function, one can write

\[
\text{Re} \chi(q, \omega) = -\lim_{\epsilon \to 0} \sum_{m,n} f_{nm}(\beta) \left| V_{nm} \right|^2 \frac{(\omega + E_n - E_m)}{(\omega + E_n - E_m)^2 + \epsilon^2},
\]

\[
\text{Im} \chi(q, \omega) = \pi \sum_{m,n} f_{nm}(\beta) \left| V_{nm} \right|^2 \delta(\omega + E_n - E_m).
\]

The corresponding real-time retarded spin-correlation function is obtained via a Fourier transformation as

\[
\chi(q, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \ e^{-i\omega t} \chi(q, \omega)
= -i \theta(t) \sum_{m,n} f_{nm}(\beta) \left| V_{nm} \right|^2 e^{i(E_n - E_m)t},
\]

where \( \theta(t) \) is the Heaviside function.

To determine the correlation functions in frequency space we use the same methods as described in Ref. \[\ref{17}\] which we briefly summarize. At low temperatures small systems exhibit a small number of dominant spectral lines at frequencies \( \tilde{\omega} \) which usually can be attributed to specific excitations. The imaginary part of the correlation function is determined most accurately by “binning” the data as

\[
\text{Im} \chi(q_{\ast}, \tilde{\omega}_{\ast}^\text{inf} < \omega < \tilde{\omega}_{\ast}^\text{sup}) = \sum_{m,n} f_{nm}(\beta) \left| V_{nm} \right|^2 \frac{\left[ \theta(\omega_{nm} - \tilde{\omega}_{\ast}^\text{inf}) - \theta(\omega_{nm} - \tilde{\omega}_{\ast}^\text{sup}) \right]}{\tilde{\omega}_{\ast}^\text{sup} - \tilde{\omega}_{\ast}^\text{inf}}.
\]

For small systems at low temperatures the appropriate choice is such that the interval boundaries lie in the middle between the dominant spectral lines:

\[
\tilde{\omega}_{\ast}^\text{sup} = \tilde{\omega}_{\ast}^\text{inf} = (\tilde{\omega}_j + \tilde{\omega}_{j+1})/2.
\]

If only the “dominant” spectral lines are present and if those lines form a well defined continuum in the thermodynamic limit, i.e., \( \sum_{m,n} f_{nm}(\beta) \left| V_{nm} \right|^2 \to \infty \), Karbach, Müller, and coworkers have shown that Eq. \([\ref{5}]\) can be used, appropriately scaled to the thermodynamic limit, by introducing a density of states with respect to appropriate quantum numbers derived from Bethe ansatz. This leads to the following representation of the imaginary part of the correlation function:\[\ref{17}\]

\[
\text{Im} \chi(q_{\ast}, \tilde{\omega}_{\ast}) = \sum_{m,n} \frac{2\pi f_{nm}(\beta) \left| V_{nm} \right|^2}{\tilde{\omega}_{j+1} - \tilde{\omega}_j}.
\]

The sum covers only values of \( n \) and \( m \) such that \( \tilde{\omega}_j = E_n - E_m \). In Heisenberg chains this representation is only applicable at \( T = 0 \).

It can be shown that Eq. \([\ref{5}]\) gives very accurate results for the real part of the correlation function if it is determined at the dominant spectral lines \( \tilde{\omega}_j \).

\[
\text{Re} \chi(q_{\ast}, \tilde{\omega}_{\ast}) = -\sum_{m,n} f_{nm}(\beta) \left| V_{nm} \right|^2 \theta(|E_n - E_m - \tilde{\omega}_{\ast}| - \Delta \omega)
\]

The regularization parameter \( \Delta \omega \) can be set to zero if only excitations at \( \tilde{\omega}_{\ast} \) are present (define \( \theta(0) = 0 \)). For Heisenberg chains at intermediate temperatures and frequencies a choice of \( \Delta \omega = 0.1 J \) yields reliable results. For higher frequencies the results for the real part of the correlation functions are free of finite size effects.

**B. Field theoretical preliminaries and transformations**

The correlations described by \( \chi(q, \omega) \) Eq. \([\ref{5}]\) are dominant at \( q = \pi \) reflecting the antiferromagnetic instability of the system. We will thus focus on this wave vector. For \( q \sim \pi \) and \( J_2 = 0 \) the spin-correlation function has been studied in detail with bosonization techniques by Schulz \([\ref{13}]\) and has later been improved including logarithmic corrections \[\ref{14}\]. The result of conformal field theory for any two-point function with scaling dimension \( x \) in Euclidean space \((r, \tau)\) at low temperature \( T \) is

\[
\chi_{\text{CFT}}(r, \tau) = \chi_0 \left[ \frac{\pi T}{v} \frac{\pi T}{\sinh \pi T (\frac{r}{v} + i \tau)} \frac{\pi T}{\sinh \pi T (\frac{r}{v} - i \tau)} \right]^x,
\]

where \( v \) denotes the velocity of the low lying spin excitations, and \( \chi_0 \) is some constant. The spin wave velocity for frustrated Heisenberg chains has been determined numerically as \( v = 0.5 \pi (1 - 1.12 J_2) \) for \( J_2 < 0.2411 \). The Fourier representation in momentum \( q \) and frequency \( \omega \) space with \( \text{Im} \omega > 0 \) is

\[
\chi_{\text{CFT}}(q, \omega) = \sin(\pi x) \frac{v^{1-2x}}{2 \pi T} \chi_0 (\pi T)^{2x-2} F_x \left( \frac{\omega - v(q - \pi)}{2 \pi T} \right) F_x \left( \frac{\omega + v(q - \pi)}{2 \pi T} \right)
\]

with

\[
F_x(k) = \int_0^\infty d\lambda \left( \frac{\sinh \lambda}{\sinh \lambda^x} \right)^x = 2^{x-1} \Gamma(1 - x) \frac{\Gamma(x/2 - ik/2)}{\Gamma(1 - x/2 - ik/2)}.
\]
From this representation we learn that the function on the right hand side of Eq. (14) is analytic in a strip around the real axis with \(|\text{Im } \omega| < x \pi T\) as long as \(T > 0\); for \(T = 0\) we have

\[
\text{Im } \chi_{\text{CFT}}(q, \omega) \simeq \begin{cases} 
0, & \text{for } \omega < \omega(q - \pi) \\
\frac{\exp(-x \pi T t)}{t^{1-2x}}, & \text{for } T > 0 \text{ and } q = \pi, \\
\frac{\exp(-x \pi T t)}{t^{1-2}}, & \text{for } T = 0.
\end{cases} 
\] (16)

These analytical properties are shared by the structure factor \(S_{\text{CFT}}(q, \omega)\), which is related to \(\text{Im } \chi_{\text{CFT}}(q, \omega)\) via Eq. (3), i.e., it is analytic in \(|\text{Im } \omega| < x \pi T\) for \(T > 0\), and \(S_{\text{CFT}}(\pi, \omega) \simeq \omega^{-2} \pi^{-2} \text{ for } T = 0\).

Performing the Fourier transform to real time we see that both \(\chi_{\text{CFT}}(q, t)\) and \(S_{\text{CFT}}(q, t)\) decay exponentially at finite temperatures and algebraically for \(T = 0\) and \(q = \pi\),

\[
\chi_{\text{CFT}}(\pi, t) \simeq \exp(-x \pi T t), \quad \text{for } T > 0 \\
\text{Im } \chi_{\text{CFT}}(q, \omega) \simeq \begin{cases} 
0, & \text{for } \omega < \omega(q - \pi) \\
\frac{\exp(-x \pi T t)}{t^{1-2x}}, & \text{for } T > 0 \text{ and } q = \pi, \\
\frac{\exp(-x \pi T t)}{t^{1-2}}, & \text{for } T = 0.
\end{cases} 
\] (17)

For momenta \(q \neq \pi\) the function \(\chi_{\text{CFT}}(q, t)\) decays exponentially with time \(t\) for any \(T > 0\) as well as \(T = 0\).

There are additional contributions to \(\chi(q, \omega)\) and \(S(q, \omega)\) on the lattice that are singular at finite values of \(\omega\) even for \(T > 0\). These contributions have their origin in the existence of the lattice which leads to finite energy bands with upper band edge singularities. There are no universal predictions like for the lower band edge governed by conformal field theory and described above. An exception, of course, is the XY spin model which can be mapped to free fermions.

As we discuss in Sec. II C the case of the XY model suggests to assume that \(\chi(q, \omega)\) is singular at a frequency \(\Lambda\) where the imaginary part diverges like

\[
\text{Im } \chi(q, \omega) \pm i \epsilon = \begin{cases} 
\pm (\Lambda - \omega)^{\alpha}, & \text{for } \omega < \Lambda \\
0, & \text{for } \omega > \Lambda.
\end{cases} 
\] (18)

The upper (lower) sign yields the retarded (advanced) correlation function. If not stated explicitly we discuss the retarded functions. The Kramers-Kronig transform yields the singularity of the real part

\[
\text{Re } \chi(q, \omega) = \begin{cases} 
\cot \pi \alpha (\Lambda - \omega)^{\alpha}, & \text{for } \omega < \Lambda \\
\frac{\text{sign}(\omega)}{\sin \pi \alpha} (\omega - \Lambda)^{\alpha}, & \text{for } \omega > \Lambda.
\end{cases} 
\] (19)

In the neighborhood of \(\alpha = 0\) we have a logarithmic singularity

\[
\text{Re } \chi(q, \omega) = \frac{\text{sign}(\omega)}{\pi} \ln |\Lambda - \omega|.
\] (20)

Regarding the time dependence we note that both functions \(\chi(q, t)\) and \(S(q, t)\) are dominated by the singularity at \(\Lambda\) and show long time asymptotics

\[
\chi(q, t) \simeq t^{-(1+\alpha)} \exp(-i \Lambda t).
\] (21)

Since the operator \(S^z\) is self adjoint \(\text{Im } \chi(\pi, \omega)\) is odd in \(\omega\). In general we thus set \(\text{Im } \chi(\pi, \omega) \sim \text{sign}(\omega) (\Lambda^2 - \omega^2)^{\alpha}\). The Fourier transform \(\text{FT} [\chi(\pi, \omega)]\) is consequently identical to twice the sine transform of \(\text{Im } \chi(\pi, \omega)\) and \(\chi(\pi, t)\) is real. For the XY case with \(\alpha = -1/2\) we like to note more explicitly the qualitative result

\[
\text{Im } \chi(\omega \pm i \epsilon) = \begin{cases} 
\pm \frac{\text{sign}(\omega)}{\sqrt{\Lambda^2 - \omega^2}}, & \text{for } |\omega| < \Lambda, \\
0, & \text{for } |\omega| > \Lambda.
\end{cases}
\] (22)

with Kramers-Kronig transform

\[
\text{Re } \chi(\omega) = \begin{cases} 
\frac{\arcsinh \sqrt{\omega/\Lambda}}{\sqrt{\Lambda^2 - \omega^2}}, & \text{for } |\omega| < \Lambda, \\
0, & \text{for } |\omega| > \Lambda.
\end{cases}
\] (23)

For overcritical frustration \(J_2 > J_c = 0.2411\) the Heisenberg chain exhibits a gapped spectrum with a lower bound \(\Omega_g\). Considering square root divergences at the lower and upper edge of the spectrum

\[
\text{Im } \chi(\omega \pm i \epsilon) = \begin{cases} 
\pm \frac{\text{sign}(\omega)}{\sqrt{(\omega^2 - \Omega_g^2)/(\Lambda^2 - \omega^2)^2}}, & \text{for } \Omega_g < |\omega| < \Lambda, \\
0, & \text{else}.
\end{cases}
\] (24)

we obtain the Kramers-Kronig transform

\[
\text{Re } \chi(\omega) = \begin{cases} 
0, & \text{for } \Omega_g < |\omega| < \Lambda, \\
\pm \frac{\text{sign}(\omega)}{\sqrt{(\omega^2 - \Omega_g^2)/(\Lambda^2 - \omega^2)^2}}, & \text{else}.
\end{cases}
\] (25)

The upper band edge singularities and the resulting algebraic real-time asymptotics exist only at sufficiently low temperatures. At intermediate temperatures the upper limit of the continuum yields an anti-symmetrized Lorentzian contribution.

\[
\text{Im } \chi(q, \omega) \simeq L_-(\phi) - L_+(\phi),
\] (26)

where

\[
L_\pm = \frac{\Gamma \cos \phi - (\Lambda \pm \omega) \sin \phi}{\Gamma^2 + (\Lambda \pm \omega)^2 \sin^2 \phi}.
\] (27)

Limiting \(0 \leq \phi \leq \pi/2\) the real part is simply given by

\[
\text{Re } \chi(q, \omega) \simeq L_-(\phi - \pi/2) + L_+(\phi - \pi/2)
\] (28)

and the Fourier transform reads

\[
\chi(q, \omega) \simeq e^{-\Gamma t} \sin(\Lambda t + \phi).
\] (29)

This temperature range will be referred to as "diffusive regime".

C. XY model

We demonstrate the overlap of the accurate short time scale results from the exact diagonalization of finite systems and the asymptotic behavior accessible by field theory for an exactly solvable case, the XY model, where
J_{2} = J_{z} = 0. The spin operators in this model can be transformed to non-interacting spinless fermions via a Jordan-Wigner transformation. The structure factor Eq. (3) can be given for $L \to \infty$ in closed form. The imaginary part of the susceptibility at $q = \pi$ is

$$\text{Im} \chi_{XY}(\pi, \omega) = \tanh(\beta\omega/4) \left(4 - \omega^{2}\right)^{-0.5}$$  \hspace{1cm} (30)

This is the field theoretical result Eq. (14) with scaling dimension $x = 1$ multiplied with the square root divergence at the upper band edge. The limit of $T \to 0$ is given by Eqs. (22) and (23).

Fig. 1(a) shows the imaginary part of the susceptibility. The full line represents the exact results, the symbols are obtained via Eq. (11), and the step functions are given by Eq. (6). The dashed line is the result from field theory with upper band edge cutoff but without divergence. The lines in (b) are the Kramers Kronig transforms of the imaginary part, and the symbols are obtained using Eq. (12) with $\Delta \omega = 0$.

We conclude that the multiplicative approach of the low energy description from field theory with the high energy behavior is adequate. Also, the numerical approaches give a reasonable approximation to the exact result. The values of the real part for $\omega > \Lambda$ show only very little finite size effects. The divergences of the real and the imaginary part at the upper band edge show the correspondence predicted by Eqs. (22) and (23).

The retarded, real-time correlation function can be determined numerically in the thermodynamic limit.

$$\chi(q, t) = i\theta(t) \lim_{L \to \infty} \frac{1}{L} \sum_{k} (f_{k} - f_{k+q}) e^{i(E_{k} - E_{k+q})t}$$  \hspace{1cm} (31)

The energy dispersion is given by $E_{k} = J \cos k$, $f_{k}$ are Fermi distribution functions, and the sum covers the first Brillouin zone. In general for $L \geq 10^4$ the result is independent of $L$ for all practical purposes.

In Fig. 2 we show the retarded spin-correlation function for finite systems compared with the result in the thermodynamic limit ($L \to \infty$, full lines) at $T = 0$ (a) and at $T = 0.3$ (b). The different broken lines show the deviation of results for finite systems Eq. (8). $L = 14$ yields a good representation of the correlation function up to $t \approx 2J/t = 0$ and up to $t \approx 8J/t = 0.3$. The thin lines show the asymptotic behavior as predicted in Sec. II.

D. Technical outline of the approach

Renormalization group studies show that the XY model is one point of the line of critical fixed points towards which the interaction flows in a bosonized repre-
sentation of the Heisenberg model \( (J_z = 1) \). One thus expects qualitatively similar results for the unfrustrated Heisenberg chain as in the \( XY \) model. This should also hold for frustrated Heisenberg chains, at least for undercritical \( J_2 \leq J_z = 0.2411 \).

The discussion of the \( XY \) model implies that the representation of the imaginary part of the correlation function is best achieved by multiplying the upper band edge behavior to the field theoretical expression.

\[
\text{Im} \chi(\pi, \omega) = \text{Im}[\chi_{\text{CPT}}(\pi, \omega)] \left( \frac{\Lambda^2 - \omega^2}{2 \Lambda^2} \right)^{\alpha} \theta(\Lambda - |\omega|)
\]

(Eq. (32))

The real part of the susceptibility is given by the real-time representation of the Heisenberg model. This should also hold for frustrated Heisenberg chains, at least for undercritical \( J_2 \leq J_z \). The scaling variable \( \pi \) determines the critical behavior to the field theoretical expression.

The discussion of the \( XY \) model implies that the representation of the imaginary part of the correlation function is best achieved by multiplying the upper band edge behavior to the field theoretical expression.

\[
\text{Im} \chi(\pi, \omega) = \text{Im}[\chi_{\text{CPT}}(\pi, \omega)] \left( \frac{\Lambda^2 - \omega^2}{2 \Lambda^2} \right)^{\alpha} \theta(\Lambda - |\omega|)
\]

(Eq. (32))

The real part of the susceptibility is given by the real-time representation of the real part in finite systems. (a) low temperature finite size effects and thermodynamic limit values as extracted from the finite size scaling represented in (b). (c) Temperature dependence.

**FIG. 3.** First moment of the spin susceptibility as extracted from the susceptibilities of the real part in finite systems. (a) low temperature finite size effects and thermodynamic limit values as extracted from the finite size scaling represented in (b). (c) Temperature dependence.

\[
I_1(q, T) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \omega \text{Im} \chi(q, \omega)
\]

(Eq. (33))

II. SUM RULES AND PREFACTORS

Since the imaginary and real representation of the spin-correlation function are Kramers Kronig related and as a consequence of the bounded excitation spectrum \( \omega \) it is straightforward to find that the sum rule Eq. (33) is given by

\[
I_1(q, T) = -\lim_{\omega \to \infty} \omega^2 \text{Re} \chi(q, \omega).
\]

(Eq. (34))

For \( \lim_{T \to 0} I_1(q, T) = 4K_1(q) \) the structure factor sum rule discussed in Ref. [3] is reproduced. For arbitrary frustration \( J_2 \) the structure factor sum rules are connected to the ground state energy \( E_G \) of the system via \( K_1(\pi)/2 + K_1(0.5\pi) = 2E_G/3 \). We recall that for \( J_2 = 0 \) and \( J_2 = 0.5 \) one has \( K_1(q) = 2(1 - \cos q)E_G/3 \). For \( J_2 = 0.5 \) the average \( \langle S_i^zS_{i+1}^z \rangle = 0 \) vanishes.

The crucial point is that \( \text{Re} \chi(q, \omega \to \infty) \) depends only weakly on the system size \( L \). Figure 3(c) shows \( I_1(q, T) \) as a function of temperature for different system sizes and frustration parameters. In Fig. 3(a) it becomes obvious that the result for \( J_2 = 0 \) and \( L = 14 \) is for all practical purposes in the thermodynamic limit for \( T > 0.3 \). Analyzing Eq. (13) one finds the correlation length to be \( \xi = \nu/(2\pi x T) \). For \( x \approx 0.5 \) and \( \nu = 0.5\pi(1 - 1.12J_2) \) we find that the finite size effects are of the order of \( 10^{-3} \) when the correlation length becomes \( \xi > L \).

Figure 3(b) shows the values of \( I_1(\pi, 0) \) as a function of the system size. We determine the thermodynamic limit with the algebraic scaling function \( I_1(\pi, 0, L) = I_1(\pi, 0, \infty) + A_0 L^{-\eta} \). Systems with \( L \) odd \( 4 \) and \( \nu = 0.5\pi(1 - 1.12J_2) \) we find that the finite size effects are of the order of \( 10^{-3} \) when the correlation length becomes \( \xi > L \).

In Fig. 3(a) the peculiar finite size effects for \( J_2 = 0.45 \) becomes apparent. Obviously they result from the gap values of \( \Omega_1 \approx 0.12 \) being just in the temperature range where the finite size effects appear. The determination of \( I_1(\pi, 0) = 1.075(10) \) is thus less accurate. The results are represented by the symbols in Fig. 3(a).
In Fig. 3(c) the temperature dependence of $I_{1}(\pi, T)$ is shown for different values of the frustration parameter. The general asymptotic behavior of $\lim_{T \to \infty} \chi(\pi, \omega) \sim T^{-1}$ becomes apparent from the discussion in section III. For the first moment we find $\lim_{T \to \infty} I_{1}(\pi, T) = 0.5/T$. This is reminiscent of the structure factor sum rule

$$\lim_{\omega \to \infty} T^{2} \omega^{2} \text{Re} \chi(\pi, \omega) = \lim_{T \to \infty} \int_{-\infty}^{\infty} d\omega' \omega'^{2} S(\pi, \omega') = 0.5$$

and is generic for all values of $J_{2}$ and the XY model. Note that $\lim_{T \to \infty} S(q, \omega) = \lim_{T \to \infty} S(q, -\omega)$.

The values of $\text{Re} \chi(\pi, \omega = 0)$ show little finite size effects even at rather low temperatures. Figure 4 shows a Log-Log plot from Eq. (4) for different values of the frustration $J_{2}$ and chain lengths as a function of temperature (broken lines). The full line shows the asymptotic behavior

$$\lim_{T \to \infty} T \text{Re} \chi(\pi, 0) = \lim_{T \to \infty} \int_{-\infty}^{\infty} d\omega' S(\pi, \omega') = 0.25$$

which reproduces a structure factor sum rule and is identical for all values of the frustration and the XY model.

The field-theoretical prediction Eq. (14) for the prefactor $T^{2} \omega^{2}$ with constant scaling variable $x$ is clearly inappropriate for the temperature range shown. Our analysis in Sec. III shows that the deviation results from an explicit temperature dependence of the singularity at the upper band edge, i.e., $\Lambda(T)$ and $\alpha(T)$.

The inset of Fig. 4 shows the finite size effects at low temperatures. $\lim_{T \to \infty} \text{Re} \chi(\pi, \omega = 0)$ diverges for $J_{2} \leq 0.2411$ and saturates for $J_{2} > 0.2411$ which is reminiscent of the presence of a gap.

For completeness we show in Fig. 5 the temperature dependence of $\text{Re} \chi(\pi, 3.8)$ from Eq. (14) for different values of $J_{2}$. The finite size effects are $\leq 0.1\%$ and hardly visible on this scale (full lines $L = 14$, broken lines $L = 12$). We do not show plots for $J_{2} = 0.5$ since the presence of bound states makes the result unreliable, c.f. section III.C.

III. FRIUSTRATED HEISENBERG CHAINS

We now turn to the determination of line shapes of the spin-correlation function in frustrated Heisenberg chains making use of the precise results obtained above.

A. Critical frustration

We first discuss the values of $J_{2} = 1$ and $J_{2} = J_{c}$ at the quantum critical point making the field-theoretical results eligible for comparison. In frequency space at $T = 0$

for a 14 site chain there are four spectral lines at frequencies $\omega_{j} \in W^{(14)} = \{0.264, 1.309, 2.112, 2.437\}$ which, by analogy to the dimer-dimer correlation functions, may be identified as the triplet excitations out of the ground state. It is thus reasonable to suppose them to form a well defined continuum in the thermodynamic limit and thus Eqs. (11) and (12) can be applied with $\Delta\omega = 0$.

The imaginary part of the spin-correlation function is $\chi$ out of the ground state. The full line is the universal large $T$ asymptotic result $\sim 0.25/T$. The inset shows the finite size effects at low temperatures. $\lim_{T \to \infty} \text{Re} \chi(\pi, \omega = 0)$ diverges for $J_{2} \leq 0.2411$ and saturates for $J_{2} > 0.2411$.

For completeness we show in Fig. 5 the temperature dependence of $\text{Re} \chi(\pi, 3.8)$ from Eq. (14). The finite size effects are $\leq 0.1\%$ and hardly visible on this scale (full lines $L = 14$, broken lines $L = 12$).
FIG. 6. Imaginary part (a) and real part (b) of the spin-correlation function in the frustrated Heisenberg chain at $T = 0$ with $J_2 = 0.2411$. The imaginary part for finite systems is binned (Eq. (4)), each bin holds one spectral line, symbols are from Eq. (11). The symbols for the real part are obtained by using Eq. (12). The full lines are the theoretical result from Eq. (2) and its KKT. Inset: enlargement of cutoff region with finite size results from Eq. (4).

FIG. 7. Real-time spin-correlation function for $J_2 = 0.2411$ at (a) $T = 0$ and (b) $T = 0.3$. Broken lines are finite size data from Eq. (8), full lines are FT of Eq. (12).

the correlation function up to $t \approx 2/J$.

The fit with the theoretical predictions from Eq. (12), its KKT, and FT are given by the full lines in Figs. 7(a), 7(b), and 7(a) using the parameter set $p_{0.2411}(0) = (0.50(1), 2.6(1), -0.10(7))$. The cutoff $2.5 < \Lambda$ is bound by the highest spectral lines which must lie in the continuum. Previous results suggest $\Lambda$ to decrease monotonously with temperature and for reasons of consistency $\Lambda < 2.7$. The three parameters are then determined by matching the first maximum as well as the slope for $1 < tJ < 2$ in the real time representation and the value of the real part for $\omega \sim 3.8$ (c.f. Fig. 5). The finite size effects require to allow for rather large error margins.

The result of $x$ is consistent with the prediction from field theory. The value of $\alpha \neq 0$ suggests a more complicated upper continuum edge than a simple ultraviolet cutoff. We emphasize that the overall prefactor of the fit function is fixed by the sum rule Eq. (32) and that values for $\Lambda$ and $\alpha$ have been obtained without using the not so well defined binned data of the imaginary part.

The plot of the real-time representation of the spin-correlation function at $T = 0.3$ in Fig. 7(b) reveals the temperature dependence of the parameter vector $p_{0.2411}(0.3) = [0.48(1), 2.5(1), -0.25(5)]$. The result for $L = 14$ yields a useful representation of the correlation function up to $t \approx 4/J$. The full line is the fit from the FT of Eq. (12). The exponential fall off predicted in Sec. 79 is confirmed and renders the value of the scaling dimension. The oscillations are much less damped than would be obtained with an upper band edge exponent of $\alpha = 0$ thus yielding the negative value of $\alpha = -0.25$. The cutoff $\Lambda$ is given via the period of the oscillations.

FIG. 8. Imaginary part (a) and real part (b) of the spin-correlation function in the frustrated Heisenberg chain at $T = 0.3$ with $J_2 = 0.2411$. The imaginary part for finite systems is binned (Eq. (4)), the symbols for the real part are obtained using Eq. (12). The full lines are the theoretical result from Eq. (12) and its KKT. Inset: enlargement of cutoff region with finite size results from Eq. (4).
14 they are given by the frequencies $\tilde{\omega}_j \in \mathcal{V}^{(14)}_{\lambda} = \{0.311, 0.971, 1.517, 2.068, 2.301\}$. The condition of a well defined continuum with respect to Bethe ansatz quantum numbers is violated and thus Eq. (13) cannot be applied any more. For the real part the data are regularized with $\Delta \omega = 0.1$, which is determined to give reliable results analogously to the dimer-dimer correlation functions. An exception is made at $\omega = 0$, where no regularization is applied ($\Delta \omega = 0$).

The good correspondence of the field-theoretical fits from Eq. (13) and its KKT (solid lines) in Figs. 8(a) and 8(b) proves the reliability of the parameters extracted from the real-time representation. Especially the good agreement of the values of Re $\chi(\pi,0)$ and of Re $\chi(\pi,\omega > 2.7)$ (inset Fig. 8(b)) are non-trivial consistency checks. We expect a thermal smearing out of the small divergence at the upper band edge of which the shape is not known and which we did not account for (solid line in Fig. 8(a)). This might have a small influence on the parameters extracted and thus we adapted rather conservative error bars. The finite size data in both the real and imaginary part suggest a steeper slope in the low frequency dependence of the fitted curves. Together with the temperature dependence of the scaling dimension $\chi$ this indicates the breakdown of the scale invariance predicted by field theory at finite temperatures.

B. Unfrustrated Heisenberg chain

Heisenberg chains without frustration are relevant for most of the magnetically quasi one-dimensional systems studied experimentally. Since the system is integrable the numerical data can be compared to results from Bethe ansatz.

At $T = 0$ the four spectral lines of the triplet excitations out of the ground state for a 14 site chain are at frequencies $\tilde{\omega}_j \in \mathcal{V}^{(14)}_{\lambda} = \{0.307, 1.57, 2.56, 3.10\}$. It is thus reasonable to suppose them to form a well defined continuum in the thermodynamic limit and thus Eqs. (13) and (12) can be applied with $\Delta \omega = 0$. Binned data for the imaginary part are obtained via Eq. (14).

The imaginary part of the spin-correlation function is shown in Fig. 9(a). The real part in Fig. 9(b) shows for $\omega = 0$ significant finite size effects since Re $\chi(T=0)|_{\pi,\omega=0} \rightarrow \infty$. For $\omega > 3.5$ the numerical results are essentially in the thermodynamic limit (Inset of Fig. 9(b)). The real-time representation of the spin-correlation function at $T = 0$ is given in Figure 10(a).

The upper edge of the two-spinon continuum is known exactly to be $\lambda = \pi$. Bethe ansatz results suggest that the infra red divergence of the two-spinon contribution $\chi(2)$ to the imaginary part of the spin-correlation function has a logarithmic correction

$$\lim_{|\omega| \rightarrow 0} \text{Im} \chi(2)(\pi,\omega) \propto \omega^{-1} \sqrt{\ln(\omega^{-1})}$$

while at the upper continuum edge it vanishes square root like. The two-spinon contribution has been found to contribute $72.89\%$ to the total spectral weight. Our and previous numerical studies show that the spectral weight of the total correlation function for above the two-spinon continuum ($\omega > \pi$) at $g = \pi$ is less than $0.1\%$. Thus the total spin-correlation function includes also about $27\%$ higher order contributions and we have Im $\chi(\pi,\omega) < \chi(2)(\pi,\omega)$. Consequently we must require $x \leq 0.5, \alpha \leq 0.5$, and $\Lambda = \pi$.

From the amplitude in the real-time representation in

![Figure 9](image-url) Imaginary part (a) and real part (b) of the spin-correlation function in the unfrustrated Heisenberg chain at $T = 0$. The binned curves in (a) are from (Eq. (14)), the symbols for the real part (b) are obtained using Eq. (14). The full lines are the fits from Eq. (13) and its KKT. Inset: enlargement of cutoff region with finite size results from Eq. (14).

![Figure 10](image-url) Real-time spin-correlation function for $J_2 = 0$ at (a) $T = 0$ and (b) $T = 0.3$. Broken lines are finite size data from Eq. (14), full lines are FT of Eq. (12).
Fig. 10 (a) we find that the parameters $x$ and $\alpha$ fall on a line defined by $0.38 < x \alpha < 0.44$. Taking also the value of the real part at $\omega = 4$ in the inset of Fig. 10(b) into consideration we determine $p_0(0) = [0.40(3), \pi \pm 0.01, 0.33(5)]$. The error margins have been chosen rather large because of the obvious finite size effects. The resulting fits with the theoretical predictions from Eqs. (12), its KKT, and FT are given by the full lines Figs. 10(a), 10(b), and 11(a) and show satisfactory agreement with the results from finite systems.

The short-dashed line in Fig. 10(b) shows the correlation function for 14 sites in the real-time representation. In the case of overcritical frustration the spectrum of the bound state contributions since results of the real-time representation are more reliable anyway.

At $T = 0$ there are more spectral lines present than in the case of critical and undercritical frustration. Some of them are signatures of the bound states present in the system. We still apply Eqs. (11) and (14) to extract the imaginary part of the spin-correlation function as shown in Fig. 12(a). The fluctuations of the results at the upper band edge are reminiscent of the fact that the bound states do not form a continuum in the thermodynamic limit. We do not attempt to refine the plot by extracting the bound state contributions since results of the real part and especially the real-time representation are more reliable anyway.

Fig. 12(b) shows the real part from Eq. (13) with $\Delta \omega = 0.1$ for $1.5 < \omega < 2.3$ and $\Delta \omega = 0.001$ else. The binned continuum one expects a density of states that diverges square root like both at the lower as well as at the upper edge. Previous numerical and variational results suggest sharp maxima in the density of states just above the lower edge $\Omega_g$ and just below the upper edge $\Lambda$ of the continuum accompanied by a square root like vanishing at both edges. This can be understood in connection with bound states being present close to the edge of the continuum.

C. Overcritical frustration

In the case of overcritical frustration the spectrum of the spin chains acquires a gap $\Omega_g$. We discuss here the value of $J_s = 0.5$ for better comparability with results from literature. For a two particle (spinon)
While the simple functional form of Eq. (32) is insufficient, the large value of $\chi_\alpha g$ requires the large value of $\Delta = 2 \Lambda$. The full line in Fig. 13(a) shows the fit from the FT of Eq. (32). The full lines in Fig. 12(a) and 12(b) show the fit of Eqs. (24) and (25) where $\chi_{\alpha g}(\pi, \omega, g) = 0$. Correspondingly, the fits to the imaginary- and the real-part representations in Fig. 14(a) and 14(b) show inconsistencies with the numerical data.

D. Intermediate temperatures

At intermediate temperatures the interaction in the system is expected to broaden out all sharp features in the correlation functions. The onset of this effect is already observed at $T = 0.3$ as discussed in the previous sections. At $T = 0.7$ the exponent of the upper continuum edge for $J_2 = 0$ is $\alpha = 3.2(1)$ so that the singularity is basically completely damped out. Also, the rather large effective continuum edge $\Lambda = 3.45(10)$ does not quite reproduce the correct oscillatory behavior as a function of time.

At about the same temperature the scaling dimension increases to $x \sim 1$. $T^* \approx 0.7$ thus marks the crossover temperature from strongly interacting, conformally invariant to noninteracting fermion and high energy diffusive behavior. This is consistent with $\partial T \text{Re } \chi(\pi, \omega)$ and $\partial T \text{Re } \chi(\pi, 3.8)$ being extremal at $T \approx T^*$ as seen in Figs. 13(b) and 14(b).

Figure 15(c) shows the real-time representation of the spin-correlation function of the unfrustrated Heisenberg chain at $T = 1$. The amplitude of the modulations between $tJ = 2$ and the onset of finite size effect for the 14 site chain at $tJ \sim 7$ cannot be fitted algebraically. The exponential fit from Eq. (24) shown by the full line in Fig. 15(c) matches excellently. The analogy to the XY model suggests that the long time asymptotics is cap-
The susceptibility for different values of the frustration in the limit of infinite temperatures. The data of the imaginary part (a) are binned and the real part (b) is given by Eq. (6) with $\epsilon = 0.02$ was applied, and in (c) Eq. (8). The solid line in (c) is the sinusoidal fit for the example of $J_2 = 0$.

In Fig. 16(a), 16(b), and 16(c) we show the respective imaginary, real, and real-time representation of the susceptibility for $T \to \infty$. Broken lines in (a) are binned, in Eq. (1) with $\epsilon = 0.02$ for $L = 14$. The time representations (c) from Eq. (8) show finite size effects for $t > 6/J$.

For $\omega \to 0$ the slopes of the imaginary part are similar to the exact result for the $XY$ model Eq. (30). A small frustration dependence becomes obvious when plotting the structure factor instead of the correlation function. The oscillations in time shown in Fig. 16(c) can be fitted very accurately for $1.5 < 2J < 6$ with an exponential decay via Eq. (29). The parameter sets $[\Lambda, \Gamma, \phi]$ are obtained as $[2.15(1), 0.375(2), -0.87(1)]$ for $J_2 = 0$, $[2.31(1), 0.323(2), -1.13(1)]$ for $J_2 = 0.2411$, and $[2.21(1), 0.345(2), -0.82(1)]$ for $J_2 = 0.5$. The full line shows the resulting fit function for $J_2 = 0$.

In the classical limit, where $\langle S_0^2 \rangle_{T \to \infty} \to \infty$, paramagnetic behavior is expected for $T \gg J$. This leads to an expected functional dependence of the structure factor of $\lim_{T \to \infty} S_{\text{class}}(q, \omega) \sim \lim_{\epsilon \to 0} \epsilon / (\omega^2 + \epsilon^2)$. From Eq. (36) it follows that $\lim_{T \to \infty} T \Re \chi \sim \langle S_0^2 \rangle_{T \to \infty}$ which is consistent with the expected functional dependence in the classical limit.

The $XY$ model is one point of the line of critical fixed points towards which the interaction flows in a bosonized representation of the Heisenberg model Eq. (29). The susceptibility of the $XY$ model shows a square root divergence at $\omega = 2$ and $\Im \chi_{XY}(\pi, \omega > 2) \equiv 0$. The shape of the spectrum at the upper band edge observed for Heisenberg chains is thus an interaction effect. The shape of $\Im \chi(\pi, \omega \sim \Lambda)$ indeed resembles that of a Fermi distri-

**E. High temperature limit**

In Fig. 16(a), 16(b), and 16(c) we show the respective imaginary, real, and real-time representation of the sus-

**FIG. 15.** Spin-correlation function of the unfrustrated Heisenberg chain at $T = 1$. The broken line in (a) is the binned imaginary representation, the broken lines in (b) are the real part from Eq. (6) with two values of $\epsilon$ for regularization, all for $L = 14$. Full lines in (a) and (b) are double Lorentzian fits. (c) shows the real-time representation from finite systems (broken lines) and the asymptotic fit (full line) with $\Lambda = 2.31(1), \Gamma = 0.941(5)$, and $\Lambda = -0.67(5)$.

**FIG. 16.** Imaginary (a), real (b), and real-time (c) representation of the susceptibility for $T \to \infty$. Broken lines in (a) are binned, in Eq. (1) with $\epsilon = 0.02$ was applied, and in (c) Eq. (8). The solid line in (c) is the sinusoidal fit for the example of $J_2 = 0$.

The discrepancy of the real-time fit function (full line in Fig. 15(c)) and the correct line shape for small times does not allow for a direct comparison of the results with its Fourier transforms. The difference between the fit and the exact result is roughly exponential. The fit with Eq. (29) implies that the real and imaginary part should contain contributions from the continuum boundary Lorentzians Eqs. (29) and (30). Indeed, the double Lorentzian fits (full lines in Fig. 15(a) and 15(b)) with an additive Lorentzian contribution centered at $\omega = 0$ compare well with the binned data for the imaginary part and the real part data from Eq. (8) with $\epsilon = 0.03$ (broken lines). The fit parameters even though similar are not such that the fits are appropriately Kramers-Kronig lines). The fit parameters even though similar are not such that the fits are appropriately Kramers-Kronig related. The fits must thus be regarded as sophisticated guides to the eye. Similar results are obtained for $J_2 > 0$. Similar line shapes are also found in systems with large spins.

...
distribution of weakly interacting electrons. We thus interpret the limit $T \to \infty$ as best described by weakly interacting spinless fermions.

IV. RESULTS

Figure 17 summarizes as a function of the frustration $J_2$ at $T = 0$ the extracted values for (a) the sum rule $I_1(\pi, 0)$, (b) the scaling dimension $\xi$, (c) the upper edge of the continuum, and (d) the exponent at the upper edge of the continuum as a function of $J_2$ at $T = 0$.

(a) The values of $I_1$ for $J_2 \leq 0.2411$ are within error bars almost identical which underlines the common feature of Heisenberg chains with undercritical frustration.

(b) The scaling variable $x$ shows a stronger infrared divergence for unfrustrated Heisenberg chains than for those with critical frustration. The values for overcritical frustration have to be regarded as effective ones as discussed in Section III.C.

(c) The cutoff frequency of the upper limit of the spinon continuum is linear as a function of frustration for $J_2 < 0.35$.

(d) The exponent of the cusp at the upper boundary of the spinon continuum is always smaller than the value of $\alpha = 0.5$ predicted for the two-spinon contribution for $J_2$. The value of $\alpha$ vanishes for $J_2 \approx 0.2$ in agreement with the previous observation that for that value the spectral properties of the frustrated Heisenberg chain are similar to the conformally invariant Halpern-Shastry model.

The prefactor $\chi_0$ from Eq. (14) is of order 1 and slightly frustration dependent. The values $(J_2, \chi_0)$ are: $(0, 1.31(5))$, $(0.15, 1.12(5))$, $(0.2411, 1.01(5))$, and $(0.35, 0.88(5))$. For $J_2 = 0.5$ one has $v^{1-2x}\chi_0 = 0.69(5)$. Values for $J_2 = 0.45$ are not computed because of the peculiar finite size effects shown in Figure 3.

Figure 18 summarizes the temperature dependence of the fit parameters for the experimentally most relevant unfrustrated chain with $J_2 = 0$.

(a) The scaling variable approaches the value of the $XY$ model limit at the crossover temperature to the diffusive regime $T^* \approx 0.7$. The direct determination of $x(T > T^*)$ is not possible but since for $T \to \infty$ the weakly interacting fermion case is recovered it is expected to lock in at $x(T > T^*) = 1$.

(b) The upper continuum edge $\Lambda(T < T^*)$ marks a sharp cutoff (full symbols) while in the diffusive regime (open symbols) it is the effective, thermally smeared out upper continuum boundary. In the weakly interacting fermion limit it saturates at $\Lambda(T \to \infty) = 2.15(1)$.

(c) The exponent of the upper continuum edge $\Gamma$ increases with increasing temperature reflecting the thermal smearing out of the singularity. Its value at $T^*$ is so large that the cutoff is barely singular and thus not very well defined. In the diffusive regime ($T > T^*$) this quantity is undefined.

(d) $\Gamma$ is an effective parameter that controls the continuous transition of the system from the diffusive behavior at $T^*$ to the weakly interacting fermion limit at $T \to \infty$. For $J_2 = 0$ it saturates at $\Gamma(T \to \infty) = 0.375(2)$. 

FIG. 17. Extracted values for (a) the sum rule $I_1(\pi, 0)$, (b) the scaling dimension $\xi$, (c) the upper edge of the continuum, and (d) the exponent at the upper edge of the continuum as a function of $J_2$ at $T = 0$.

FIG. 18. Extracted values for (a) the scaling dimension $\xi$ for $T < T^*$, (b) the upper continuum cutoff frequency for $T < T^*$ (full symbols) and the effective upper continuum edge in the diffusive/weakly-interacting-fermion regime (open symbols), (c) the cutoff exponent, and (d) the control parameter $\Gamma$ determining the decay as a function of time in the diffusive/weakly-interacting-fermion regime.
V. CONCLUSIONS

We have compared numerical results from the exact diagonalization of finite systems with results from conformal field theory together with implications from the density of states, the exactly solvable XY model, and Bethe ansatz solutions for integrable systems. We use the different finite size accuracy of the imaginary, real, and temperature representations of the spin-correlation functions to extract reliable information on the thermodynamic limit.

At low temperatures the dynamical correlation functions of frustrated Heisenberg chains are well described by a multiplicative superposition of the contribution from low lying elementary excitations described by conformal field theory and a density of states and matrix element induced singularity near the upper edge of the two-spinon continuum. At the frustration value of $J_2 \approx 0.2$ the system is closest to the conformally invariant Haldane-Shastry model.

At $T^* \approx 0.7$ we observe the crossover from the low temperature, conformally invariant regime to a diffusive regime. All correlations in time then decay exponentially. The diffusive regime connects continuously to the weakly-interacting-fermion regime for $T \to \infty$.

We give the frustration dependence of the control parameters for the line shapes of the spin-correlation functions at $T = 0$ and their temperature dependence for the experimentally most relevant case of $J_2 = 0$. The temperature dependence of the first moment sum rule of the spin-correlation function is accurately determined.

VI. ACKNOWLEDGMENTS

We thank I.A. Zaliznyak, J. Stolze, V.J. Emery, and M. Weinert for stimulating and instructive discussions. The work performed at BNL was supported by DOE contract number DE-AC02-98CH10886.

1. M. Karbach and G. Müller, Comp. in Phys. 11, 36 (1997).
2. M. Karbach, K. Hu, and G. Müller, Comp. in Phys. 12, 565 (1998).
3. O. A. Starykh, A. W. Sandvik, and R. R. P. Singh, Phys. Rev. B 55, 14953 (1997).
4. K. Fabricius, U. Löw, and J. Stolze, Phys. Rev. B 55, 5833 (1997).
5. H. Yokoyama and Y. Saiga, J. Phys. Soc. Jpn. 66, 3617 (1997).
6. K. Fabricius and U. Löw, Phys. Rev. B 57, 13371 (1998).
7. G. Müller, H. Thomas, H. Beck, and J. C. Bonner, Phys. Rev. B 24, 1429 (1981).
8. H. J. Schulz, Phys. Rev. B 34, 6372 (1986).
9. A. M. Tsvelik, Quantum field theory in condensed matter physics (Cambridge University Press, Cambridge, 1995).
10. V. J. Emery and C. Noguera, Phys. Rev. Lett. 60, 631 (1988).
11. R. Chitra et al., Phys. Rev. B 52, 6581 (1995).
12. Y. Yu, G. Müller, and V. Viswanath, Phys. Rev. B 54, 9242 (1996).
13. M. Karbach et al., Phys. Rev. B 55, 12510 (1997).
14. O. A. Starykh, R. R. P. Singh, and A. W. Sandvik, Phys. Rev. Lett. 78, 539 (1997).
15. M. Karbach, K. Hu, and G. Müller, cond-mat/0008018 (unpublished) (2000).
16. M. Karbach and G. Müller, Phys. Rev. B 62, 14871 (2000).
17. R. Werner, Phys. Rev. B 63, in print (2001).
18. T. Ami et al., Phys. Rev. B 51, 5094 (1995).
19. N. Motoyama, H. Eisaki, and S. Uchida, Phys. Rev. Lett. 76, 3212 (1996).
20. R. Coldea et al., J. Phys.: Condens. Matter 8, 7473 (1996).
21. D. A. Tennant, R. A. Cowley, S. E. Nagler, and A. M. Tsvelik, Phys. Rev. B 52, 13368 (1995).
22. R. Werner, The spin-Peierls transition in CuGeO$_3$ (Ph.D. thesis, Dortmund, 1999), http://edora.de:8080/FB2/is8/forschung/1999/werner.
23. A. Fledderjohann and C. Gros, Europhys. Lett. 37, 189 (1997).
24. E. F. Fradkin, Field Theories of Condensed Matter Systems (Addison-Wesley, New York, 1991).
25. V. J. Emery, in Highly conducting one-dimensional solids, edited by J. T. Devreese, R. P. Evrard, and V. E. van Doren (Plemun, New York, 1979), p. 247.
26. K. Nomura and K. Okamoto, J. Phys. A: Math. Gen. 27, 5773 (1994).
27. The requirement of the spectrum to be bounded can be relaxed to $\lim_{\omega \to \infty} \chi(q, \omega) \sim \omega^{-s}$ with $s > 2$. For $s = 2$ there will be logarithmic corrections $\lim_{\omega \to \infty} \chi(q, \omega) \sim \omega^{-2}\ln[\omega^{-1}]$.
28. C. K. Majumdar and D. K. Ghosh, J. Math. Phys. 10, 1388 (1969).
29. Interestingly, the spectral lines from the singlet excitations relevant for the dimer-dimer correlation function and the triplet excitations are degenerate for $J_2 = J_c$.
30. For practical purposes this discrepancy can be overcome for small frequencies by rescaling the frequency dependence as has been done in the case of dimer-dimer correlation functions (see Ref. [17]).
31. J. des Cloizeaux and J. J. Pearson, Phys. Rev. 128, 2131 (1962).
32. B. S. Shastry and B. Sutherland, Phys. Rev. Lett. 47, 964 (1981).
33. G. Uhrig, Niedrigdimensionale Spinsysteme und Spin-Phonon-Kopplung (Habilitation, Cologne, 1999).
34. J. Villain, J. Phys. France 35, 27 (1974).
35. F. D. M. Haldane, Phys. Rev. Lett. 60, 635 (1988).
36. B. S. Shastry, J. Stat. Phys. 50, 57 (1988).