Quantum-critical scaling and temperature-dependent logarithmic corrections in the spin-half Heisenberg chain

O. A. Starykh, R. R. P. Singh, and A. W. Sandvik

1 Department of Physics, University of California, Davis, California 95616
2 National High Magnetic Field Laboratory, 1800 East Paul Dirac Drive, Florida State University, Tallahassee, FL 32306

(December 31, 2021)

Low temperature dynamics of the \( S = \frac{1}{2} \) Heisenberg chain is studied via a simple ansatz generalizing the conformal mapping and analytic continuation procedures to correlation functions with multiplicative logarithmic factors. Closed form expressions for the dynamic susceptibility and the NMR relaxation rates \( \frac{1}{T} \) are obtained, and are argued to improve the agreement with recent experiments. Scaling in \( q/T \) and \( \omega/T \) are violated due to these logarithmic terms. Numerical results show that the logarithmic corrections are very robust. While not yet in the asymptotic low temperature regime, they provide striking qualitative confirmation of the theoretical results.

PACS: 75.10.3m, 75.40.Gb, 75.50.Ee, 76.60.-k

In recent years there has been much interest in quantum critical phenomena in spin-models and real materials. In path integral formulations, the inverse temperature \( \beta \) acts as a finite size for the imaginary-time fluctuations, driving the system away from the \( T = 0 \) quantum critical point. The resulting behavior can be described in a manner analogous to finite-size scaling. In two-dimensions, quantum critical points are rare, but their relevance to real materials is enhanced by the fact that they also control the finite temperature properties of weakly-ordered or weakly-gapped systems [1].

In contrast to 2D, 1D quantum antiferromagnets with continuous symmetry are generically critical at \( T = 0 \). Thus one expects to find many examples of quantum critical phenomena in quasi-one dimensional materials. Recently, quantum critical behavior of spin-chains have been studied by neutron scattering [2] and NMR experiments [3].

From a theoretical point of view, the development of conformal field theory provides a powerful machinery to study the finite temperature correlation functions at a \( T = 0 \) critical point. Assuming a simple power-law behavior for the \( T = 0 \) correlation functions, various authors have obtained scaling forms for the dynamic structure factor at low temperatures [3,4,5]. However, it is well known that the \( T = 0 \) spin-spin correlations of the \( S = 1/2 \) chain, have multiplicative logarithmic factors due to the presence of marginally irrelevant operators [6]:

\[
S(0)S(x,t) >_{T=0} (\mathcal{D}T)^{x_2 - (ct)^2} \left( \ln \frac{\sqrt{x^2 - (ct)^2}}{r_0} \right)^{1/2}.
\]

Here \( c \) is the spin wave velocity, and \( D \) and \( r_0 \) are nonuniversal constants. These logarithmic factors also appear in the two-spinon contribution to the dynamic structure factor [7]\
\[
S^{(2)}_{zz}(q, \omega) \sim \frac{1}{\sqrt{\omega^2 - \omega_0^2}} \sqrt{\ln \frac{1}{\omega^2 - \omega_0^2}}.
\]

In this paper, we explore the effects of logarithmic factors on the finite temperature dynamics of the spin-half Heisenberg chain. We begin by considering the \( T = 0 \) equal-time correlations of a finite system. It was proposed in Ref. [1] that, in presence of logarithms, the correlations for a system of size \( L \) should have a generalized finite-size scaling form:

\[
S(0)S(x) >_{L} (-1)^z D \left( \frac{1}{Lx/L} \right)^{\sigma - d - 2 \eta} \times \left( \ln \frac{Lx/L}{r_0} \right)^{\sigma}. \tag{2}
\]

Here the universal function \( X(x/L) \) is given by \( X(x) = \frac{1}{\pi} \sin(\pi x) \) [1]. This proposition was shown to work well for the isotropic Heisenberg chain with \( \sigma = 1/2 \) [3].

In the absence of logarithmic factors, correlations at finite \( T \) are obtained from a conformal mapping of the complex plane \( z = x + i\tau \) at \( T = 0 \) to a strip infinite in the \( x \)-direction and of width \( c/T \) in the \( \tau \)-direction (\( \tau \) is imaginary time). In close analogy with \( T = 0 \) finite-size scaling, this amounts to the substitution

\[
LX(\frac{z}{L}, \frac{\tau}{L}) \rightarrow \frac{c}{\pi T} \left( \sin(\pi T(\frac{x}{c} + i\tau)) \sin(\pi T(\frac{x}{c} - i\tau)) \right)^{1/2}.
\]

We now assume that this mapping can also be performed in presence of marginal interactions. Then finite \( T \) spin correlations are given by the ansatz [2] with scaling function [8]. This can be further approximated as:

\[
S(0)S(x,\tau) >_{T} (-1)^z D \left( \frac{2\pi T}{c} \right)^{\frac{1}{2}} \left( \ln \frac{T_0}{T} \right)^{1/2} \times \left( \cosh \frac{2\pi T x}{c} - \cos 2\pi T \right)^{-2\Delta}, \tag{4}
\]

where \( T_0 = \sqrt{2\pi c/r_0} \), and an effective temperature-dependent scaling dimension appears [9]
\[ \Delta = \frac{1}{4} \left(1 - \frac{1}{2 \ln \frac{\pi T}{\xi}}\right). \]  

Equation (5) is valid for \( x \ll \xi \ln \frac{T_0}{T} \) (see expression for \( \xi \) below), and thus allows one to study correlations below and above the correlation length. An immediate consequence of this ansatz is that the correlation length acquires a logarithmic temperature dependence, in agreement with thermal Bethe ansatz calculations [12]:

\[ \xi^{-1} = \frac{\pi T}{c} \left(1 - \frac{1}{2 \ln \frac{\pi T}{\xi}}\right) \]  

We now explore further consequences of the scaling ansatz. First, the static structure factor is found to be

\[
S(q) = 2^{2\Delta+1/2}D \left(\frac{\ln T_0}{T}\right)^{1/2} \Gamma(1-4\Delta) \\
\times \text{Re} \left( \frac{\Gamma(2\Delta - i\frac{q}{\pi T})}{\Gamma(1-2\Delta - i\frac{q}{2\pi T})} \right),
\]

where \( q \) is measured from the antiferromagnetic vector \( \pi \). Note that the entire q-dependence of \( S(q) \) is due to the \( 1/\ln T \) corrections to the \( T = 0 \) value of \( \Delta = 1/4 \). Eq. (6) implies that \( S(q)/S(0) \) is no longer a universal function of \( cq/T \).

Performing Fourier transformation and analytic continuation to real frequencies [13,14], we obtain the staggered susceptibility

\[
\chi(q, \omega) = \frac{2^{2\Delta-3/2}D}{\pi T} \sin(2\pi T) \left(\frac{\ln T_0}{T}\right)^{1/2} \Gamma^2(1-2\Delta) \\
\times \frac{\Gamma(\Delta - i\frac{\omega - \omega_0}{4\pi T})}{\Gamma(1-\Delta - i\frac{\omega - \omega_0}{4\pi T})} \frac{\Gamma(\Delta - i\frac{\omega + \omega_0}{4\pi T})}{\Gamma(1-\Delta - i\frac{\omega + \omega_0}{4\pi T})}.
\]

This expression also lacks universality due to the \( \Delta \)-dependence of \( \Delta \).

Next, we discuss numerical results for the spin-half chain obtained using a “stochastic series expansion” Quantum Monte Carlo (QMC) method [13] (for systems with up to 1024 spins), and conventional high temperature expansions (HTE). Most results from the two methods agree down to \( T/J = 1/8 \). Below that temperature, we rely on QMC data alone.

We begin with the \( \omega = 0 \) susceptibility, shown in Fig. 1. The ratio \( \chi(q, 0)/\chi(0, 0) \) appears to converge towards a scaling form as the temperature is lowered, but even at \( \beta = 32 \) it is far from the universal scaling function expected in the absence of logarithms [14]. In the range \( 1/4 > T > 1/8 \) the numerical results have high accuracy, and QMC and HTE data agree very well. The deviations from scaling are clearly systematic, and well described by Eq. (6) with \( T_0 = 4.5 \). Note that the parameter \( T_0 \) should be considered an effective one. As the study of logarithmic corrections to the uniform susceptibility shows [15], the true value of \( T_0 \) may be reached only at \( T \leq 0.01 \).

Data for \( S(q) \) show substantial \( q \)-dependence, in disagreement with \( \Delta = 1/4 \) scaling predictions. However, the results are not well explained by Eq. (6) either. A possible reason is that \( S(q) \) is dominated by contributions (divergent at \( T = 0 \)) from short distances, where our asymptotic expression (4) breaks down. It is, thus, better to compare the equal-time real-space spin correlations, \( S(x) \), with the theoretical expressions. It is well known that the correlation function in addition to the dominant staggered piece has a uniform contribution, given by

\[
-\left(\frac{T}{2\pi \sinh(\pi T/\xi)}\right)^2 \text{ at finite } T \text{ [13].}
\]

It is appropriate to subtract this from the numerical data before comparing with the scaling theory. As shown in Fig. 2, our results for \( S(x) \) agree very well with Eq. (6), with \( T_0 = 4.5 \) and \( D = 0.075 \). The inset shows a comparison of the ratio of correlation functions at two temperatures. With \( T_0 \) fixed from the susceptibility data, this parameter-free agreement is quite striking. Deviation of the theoretical results at short distances is also apparent and is the reason that \( S(q) \) cannot be explained. The theoretical results also imply \( S(0) \sim (\ln \beta)^{1/2} \) and \( \chi(0, 0) \sim (\ln \beta)^{1/2} \) as \( T \to 0 \), in agreement with numerical data [14].

From Eq. (8) we can calculate the NMR relaxation rates

\[
\frac{1}{T_1} = \frac{2^{5/2-2\Delta}A_0^2(\pi D)}{\pi c} \sin(2\pi T) \Gamma(\Delta) \left(\frac{\ln T_0}{T}\right)^{1/2},
\]

\[
\frac{1}{T_{2G}} = \frac{2^{-3+2\Delta}A^2(\pi D)}{\pi c} \sin(2\pi T) \Gamma(2-2\Delta) \Gamma^2(1-\Delta) \left(\frac{\ln T_0}{T}\right).
\]

Here the integrals \( I_1(\Delta) = \int_0^\infty dx \frac{\pi}{\sinh(\pi x)} \) and \( I_2(\Delta) = 4 \int_0^\infty \frac{\Gamma(\Delta - i\pi x)}{\Gamma(\Delta + i\pi x)} \) have weak temperature dependences. In deriving Eq. (10), we have kept only the scaling part and dropped the term coming from self interactions as it is done by a factor \( T(\ln T_0)^2 \). The latter is, in any case, not correctly accounted for by the scaling theory. We find that Eq. (10) shows weaker than \( \sqrt{\ln T_0/T} \) variations with \( T \). This result is in qualitative agreement with recent measurement of \( 1/T_1 \) in \( \text{Sr}_2\text{CuO}_3 \) by Takigawa et al. [3]. Fig. 3 shows the ratio \( T_{2G}/\sqrt{T}T_1 \). In the \( T \to 0 \) limit our expressions (9) and (10) coincide with those of Sachdev [14]. However, we find that \( T = 0 \) limit of \( T_{2G}/\sqrt{T}T_1 \) is approached with infinite slope, similar to the behavior of the uniform susceptibility [13]. The behavior is consistent with the slow rise of this quantity seen for \( \text{Sr}_2\text{CuO}_3 \) around \( T = J/10 \) [3].

Numerical results for \( \chi'' \) are obtained from QMC data using the maximum-entropy (max-ent) method [17], and from HTE via the recursion method [16]. In Fig. 3, data are presented for the ratio with the full \( T_{2G} \) and with only the scaling part, where the self-term is not subtracted [18]. The two should converge in the scaling limit and
the latter should be compared with the theoretical result. Note that QMC and HTE results agree completely for $T_{2G}$; the deviations arise entirely from the analytic continuation needed to get $1/T_1$, which is more uncertain for QMC data (details of this point will be discussed elsewhere [19]). The difference between the curves based on the full $T_{2G}$ and the scaling part only of $T_{2G}$ shows that the results are not yet in the scaling limit. However, the theoretical results are supported by the convergence of the more accurate (in the temperature regime shown) HTE data to the predicted form. The presence of non-asymptotic contributions in the full $T_{2G}$ and the apparent tendency of QMC + max-ent to over-estimate $1/T_1$ explain the discrepancy in the numerical result previously reported for $T_{2G}/\sqrt{T_1}$ [19].

We also note that the experimental $1/T_1$ was found to be about 30% lower than the numerical result at $T = 300K$ [19], which is now also reconciled. Together with the good agreement found previously for $1/T_2$, without adjustable parameters [19], the spin-half chain indeed very well describes the low-frequency dynamics of Sr$_2$CuO$_3$.

The frequency-dependent quantities also do not show universality in the scaled variable $\omega/T$. For example, the imaginary part of the $q = 0$ and local ($\chi(\omega) = \int_{-}\infty^{\infty} dq/\pi \chi(q, \omega)$) susceptibility are given, respectively, by

$$
\chi''(0, \omega) = \frac{2^{2\Delta -3/2}D}{\pi T} \sin(2\pi \Delta) \left( \ln \frac{T_0}{\sqrt{2\pi T}} \right)^{1/2} \Gamma^2(1/2) \Gamma(1 - 2\Delta),
$$

$$
\times \text{Re} \left( \frac{\Gamma(\Delta + i\frac{\omega}{4\pi T})}{\Gamma(1 - \Delta + i\frac{\omega}{4\pi T})} \right) \text{Im} \left( \frac{\Gamma(\Delta + i\frac{\omega}{4\pi T})}{\Gamma(1 - \Delta + i\frac{\omega}{4\pi T})} \right). \tag{11}
$$

$$
\chi''(\omega) = \frac{2^{2\Delta -1/2}D}{c} \sin(2\pi \Delta) \left( \ln \frac{T_0}{T} \right)^{1/2} \Gamma(1 - 4\Delta)
$$

$$
\times \text{Im} \left( \frac{\Gamma(2\Delta - i\frac{\omega}{4\pi T})}{\Gamma(1 - 2\Delta - i\frac{\omega}{4\pi T})} \right). \tag{12}
$$

The $\omega$-dependence in Eq. (13) is due to the $T$-dependence of the scaling dimension. The $\omega$-independence and divergence at $\Delta = 1/4$ is an artifact of the approximations employed, and should be removed by more accurate treatment of the short-distance cut-off. Nevertheless, fixing the scaling dimension at $1/4$ implies a much weaker $T-$ and $\omega-$ dependence than predicted by [12]. Note also that we predict $\chi''(0, \omega) \sim (\ln \frac{T_0}{T})^{1/2}$ and $\chi''(\omega) \sim (\ln \frac{T_0}{T})^{3/2}$ at low temperatures.

QMC + max-ent data for the $q = 0$ susceptibility, as well as the results of Eq. (11), are shown in Fig. 1, where the value of $T_0$ is from the fit of the static susceptibility. At low frequencies the theory and the data agree and also appear to scale. At higher frequencies, there is no scaling and the deviations are qualitatively similar in that the lower temperature data is higher at higher values of $\omega/T$. The numerical data are not at low enough temperatures to explore the scaling forms at larger $\omega/T$. There are preliminary reports of measurements of these quantities by neutron scattering [20]. It would be useful to compare them with our results.

To conclude, we have studied the effects of logarithmic corrections on the finite temperature dynamic spin-correlations of the spin-half chain. Analytical expressions are developed for $\chi(q, \omega)$ by a generalized finite-size scaling ansatz. The ansatz ties together previous results, including logarithmic corrections to the correlation length, and implies a temperature dependent effective scaling dimension. Expressions obtained for the NMR relaxation rates are argued to improve the agreement with experimental data for Sr$_2$CuO$_3$ [3]. Numerical results, although not in the asymptotic low temperature regime, confirm various theoretical expressions including violation of scaling in the variables $cq/T$ and $\omega/T$. We expect these effects to diminish and scaling to be restored if the second-neighbor interactions are tuned to the point where the marginal interaction is absent [21]. We hope our calculations will provide further motivation for neutron scattering studies of quasi-one dimensional spin systems.

Support from the NSF through grant numbers DMR-9318537 (O.A.S and R.R.P.S) and DMR-9520776 (A.W.S) is gratefully acknowledged.
FIG. 1. The static susceptibility normalized to its \( q = 0 \) value. Symbols represent numerical data from high-temperature expansions (HTE) and Monte Carlo simulations (MC). Solid lines are predictions of Eq. (8) with \( T_0 = 4.5 \), and the dashed line shows the universal scaling function with \( \Delta = 1/4 \) [14]. The inset shows the QMC data over a larger range of \( \beta \) and \( cq/T \) together with the universal scaling function.

FIG. 2. Comparison of QMC data for real-space correlation functions (symbols) and Eq. (4) (solid lines) with \( T_0 = 4.5 \) and \( D = 0.075 \). The inset shows the ratio of the equal-time correlation functions at \( \beta = 16 \) and \( 32 \) compared with Eq. (4) and the expression with \( \Delta = 1/4 \) [14].

FIG. 3. The ratio \( T_{2G}/\sqrt{T_1} \) versus \( T \) from Eqs. (9) and (10). The \( T = 0 \) limit of the ratio is 1.68. The inset shows a linear variation with \( 1/\ln (\beta) \). QMC and HTE data for the ratio with full \( T_{2G} \) and with only the scaling part included are shown by the symbols.

FIG. 4. Imaginary part of the antiferromagnetic susceptibility. Lines represent Eq. (11) with parameters as in Fig. 2 and the symbols represent the QMC + max-ent data.
\[ \beta = 32 \quad \beta = 16 \quad \beta = 8 \quad \beta = 4 \]
\[ \Delta = \frac{1}{4} \]

\[ \chi(q, \omega = 0)/\chi(q=0, \omega = 0) \]

- \( \beta = 8, \text{MC} \)
- \( \beta = 8, \text{HTE} \)
- \( \beta = 4, \text{MC} \)
- \( \beta = 6, \text{HTE} \)
- \( \beta = 4, \text{HTE} \)

- Eq.(8), \( T_0 = 4.5 \)
- \( \Delta = \frac{1}{4} \)
$$\ln[(-1)^x S(x; \tau = 0)]$$

$$S(x; \beta = 16)/S(x; \beta = 32)$$

$$\Delta = 1/4$$

MC

Eq. (4)
The graph shows the relationship between $T_{2G}/(T_{1/2} T_1)$ and $1/\ln(\beta)$ for different scaling parts of $T_{2G}$, HTE and MC. The full $T_{2G}$, HTE and MC scaling parts are represented by different markers and lines.
