Quantum Critical Scaling and Temperature-Dependent Logarithmic Corrections in the Spin-Half Heisenberg Chain

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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 $1/T_1$ and $1/T_{2G}$ are obtained, and are argued to improve the agreement with recent experiments. Scaling in q/T and ω/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. [S0031-9007(96)02151-5]

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In recent years there has been much interest in quantum critical (QC) phenomena, particularly in the context of quasi-2D cuprate antiferromagnets. In field theory, finite-temperature QC behavior can be described in a manner analogous to finite-size scaling, with the inverse temperature β being the length of the system in imaginary time [1]. In nature, QC points in quasi-2D systems are rare, their relevance to real materials arising primarily from the fact that they also control the finite-temperature properties of weakly ordered or weakly gapped systems [1]. In contrast, half-integer spin chains with continuous symmetry are generically critical at $T = 0$, and thus many real quasi-1D antiferromagnets exhibit QC behavior in a wide temperature regime. The situation is, however, complicated by the presence of marginally irrelevant operators, which lead to logarithmic corrections to most observables. These corrections can be considerable, especially in the temperature regime where QC behavior is realized in quasi-1D materials, for, at low enough temperatures, interchain couplings always lead to 3D behavior.

In this Letter, we present new results for the logarithmic corrections to the finite-temperature dynamic susceptibility $\chi(q,\omega)$ of the standard spin-half Heisenberg chain. This quantity is directly accessible in neutron scattering experiments [2], and its $\omega \to 0$ limit determines the spin-lattice relaxation rate measured in NMR and nuclear quadrupole resonance [3]. We show that logarithmic corrections lead to measurable deviations from QC scaling even at very low temperatures and are important for understanding the NMR experiments.

Conformal field theory provides a powerful machinery to study the finite T correlation functions of systems with power-law correlations in the ground state, allowing for essentially exact calculations of the dynamic structure factor [4–6]. However, the spin chain problem is complicated by the marginally irrelevant operator, present in the bosonized Hamiltonian, which describes umklapp scattering between left and right movers [7,8]. This violates conformal invariance and leads to multiplicative logarithmic corrections at $T = 0$ [7]:

$$\langle S(0,0)S(x,t)\rangle_{T=0} = (-1)^x \frac{D}{\sqrt{x^2 - (ct)^2}} \times \left(\ln \frac{\sqrt{x^2 - (ct)^2}}{r_0}\right)^{1/2}. \quad (1)$$

Here c is the spin wave velocity, and D and r_0 are nonuniversal constants. Recently, this logarithmic factor was also found in the exact two-spinon contribution to the dynamic structure factor [9] and was shown to be important for understanding coupled spin chains [10].

The temperature introduces a finite cutoff c/T in the imaginary time (τ) direction of the complex plane $z = x + ic\tau$. Thus, the natural extension to finite T of the generalized finite-size scaling ansatz with logarithmic factors, which was proposed and tested at $T = 0$ in Ref. [11], is

$$\langle S(0)S(x,\tau)\rangle_T = (-1)^x D \frac{T}{cX(|z|T/c)} \times [\ln[T_0 X(|z|T/c)/T]]^{1/2}, \quad (2)$$

where the scaling function $cX(|z|T/c)/T \to |z|$ as $T \to 0$. For a given T, there is a range of $|z|$ such that $\ln(T_0/T) \gg \ln X(|z|T/c)$, and the square root of the logarithm can be expanded to $[\ln(T_0/T)]^{1/2} X^{\delta}(|z|T/c)$, $\delta^{-1} = 2\ln(T_0/T)$, up to $O[1/\ln(T_0/T)]$ corrections. Combined with the well-known conformal mapping of the infinite complex plane to the stripe, $x \pm ic\tau \to \frac{c}{\pi T} \sinh[\pi T(\frac{x}{c} \pm \tau)]$, this leads to the expression

$$\langle S(0,0)S(x,\tau)\rangle_T = (-1)^x D \frac{\sqrt{2}\,\pi T}{c} \left(\ln \frac{T_0}{T}\right)^{1/2} \times \left(\cosh \frac{2\pi T x}{c} - \cos 2\pi T \tau\right)^{-2\Delta}. \quad (3)$$

Equation (3) is valid for $x \ll \xi \ln T_0/T$, and allows us to study the spin correlations both above and below the correlation length ξ (see below). The high-energy cutoff is given by $T_0 = \sqrt{2}\,\pi c/r_0$. Note the appearance of an effective *temperature-dependent* scaling dimension

$$\Delta = \frac{1}{4}\left(1 - \frac{1}{2\ln\frac{T_0}{T}}\right), \tag{4}$$

in agreement with a number of renormalization group calculations on finite systems [8,11]. An immediate consequence of this is that the correlation length also acquires a logarithmic temperature dependence, in agreement with Bethe ansatz calculations [12,13]:

$$\xi^{-1} = \frac{\pi T}{c}\left(1 - \frac{1}{2\ln\frac{T_0}{T}}\right). \tag{5}$$

From Eq. (3) the static structure factor is found to be

$$S(q) = 2^{2\Delta+1/2} D\left(\ln\frac{T_0}{T}\right)^{1/2} \Gamma(1-4\Delta) \times \mathrm{Re}\left(\frac{\Gamma(2\Delta - i\frac{cq}{2\pi T})}{\Gamma(1-2\Delta - i\frac{cq}{2\pi T})}\right), \tag{6}$$

where q is measured from the antiferromagnetic vector π. Note that the entire q dependence of $S(q)$ is due to the $1/\ln(T_0/T)$ corrections to the $T = 0$ value of $\Delta = 1/4$. Equation (6) implies that $S(q)/S(0)$ is no longer a universal function of cq/T.

Fourier transformation and analytic continuation to real frequencies [4–6] give the staggered susceptibility

$$\chi(q,\omega) = \frac{2^{2\Delta-3/2}D}{\pi T}\sin(2\pi\Delta)\left(\ln\frac{T_0}{T}\right)^{1/2}\Gamma^2(1-2\Delta) \times \frac{\Gamma(\Delta - i\frac{\omega-cq}{4\pi T})}{\Gamma(1-\Delta - i\frac{\omega-cq}{4\pi T})}\,\frac{\Gamma(\Delta - i\frac{\omega+cq}{4\pi T})}{\Gamma(1-\Delta - i\frac{\omega+cq}{4\pi T})}, \tag{7}$$

which also lacks universality due to T dependence of Δ.

Next, we test the expressions derived above against numerical results for the spin-half chain obtained using a "stochastic series expansion" quantum Monte Carlo (QMC) method [14] (for systems with up to 1024 spins) and 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 [15]. In the range $1/4 > T > 1/8$ the numerical results have high accuracy, and the QMC and HTE data agree very well. The deviations from scaling are clearly systematic, and well described by Eq. (7) 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 [16], 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 (3) 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 $-(\frac{T}{2c\sinh(\pi T x/c)})^2$ at finite T [15]. 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. (3), 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 $S(0) \sim (\ln\beta)^{3/2}$ and $\chi(0,0) \sim \beta(\ln\beta)^{1/2}$ as $T \to 0$, in agreement with numerical data [17].

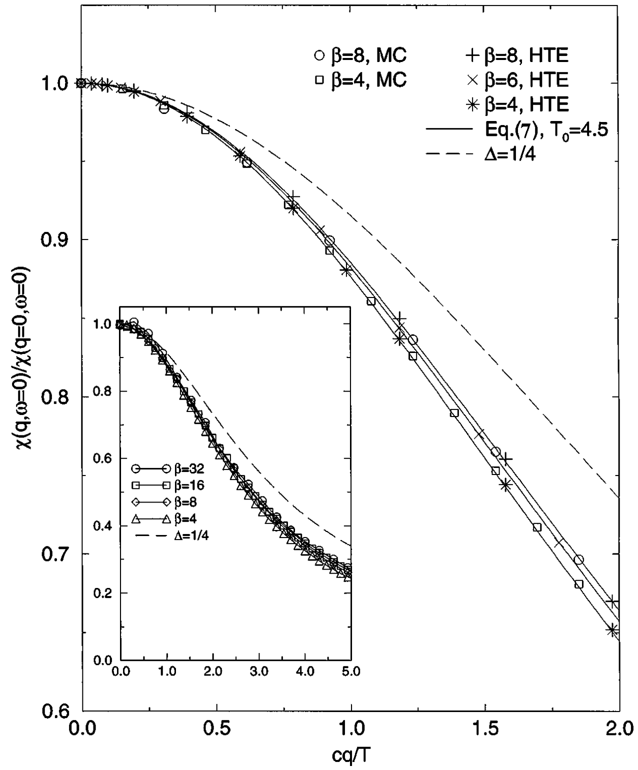

FIG. 1. The static susceptibility normalized to its $q = 0$ value. Symbols represent numerical data from high temperature expansions (HTE) and QMC simulations (MC). Solid lines are predictions of Eq. (7) with $T_0 = 4.5$, and the dashed line shows the universal scaling function with $\Delta = 1/4$ [15]. The inset shows the QMC data over a larger range of β and cq/T together with the universal scaling function.

From Eq. (7) we obtain the NMR relaxation rates [18]

$$\frac{1}{T_1} = \frac{2^{5/2-2\Delta}A_{\parallel}^2(\pi)D}{\pi c}\sin(2\pi\Delta)I_1(\Delta)\left(\ln\frac{T_0}{T}\right)^{1/2}, \tag{8}$$

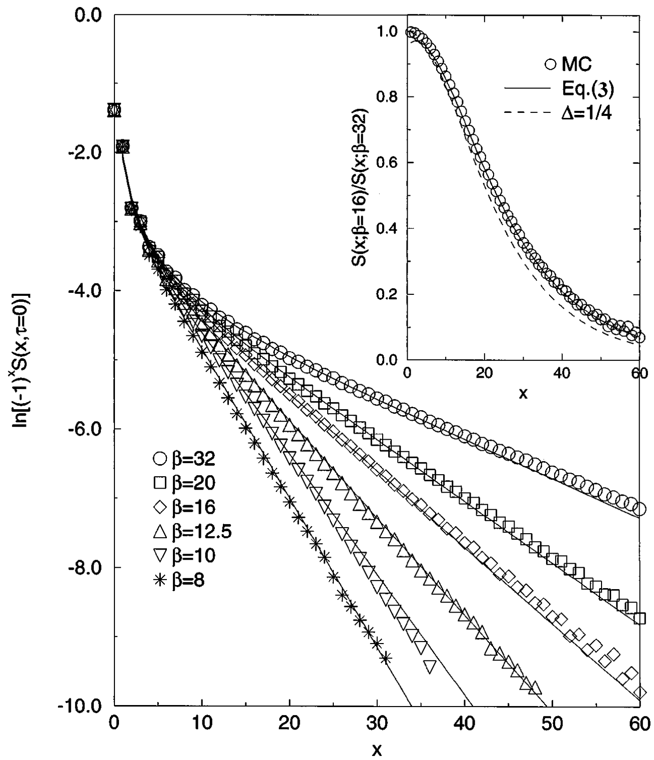

FIG. 2. Comparison of QMC data for real-space correlation functions (symbols) and Eq. (3) (solid lines) with $T_0 = 4.5$ and $D = 0.075$. The inset shows the ratio of the equal-time correlation functions at $\beta = 16$ and 32 compared with Eq. (3) and the expression with $\Delta = 1/4$ [15].

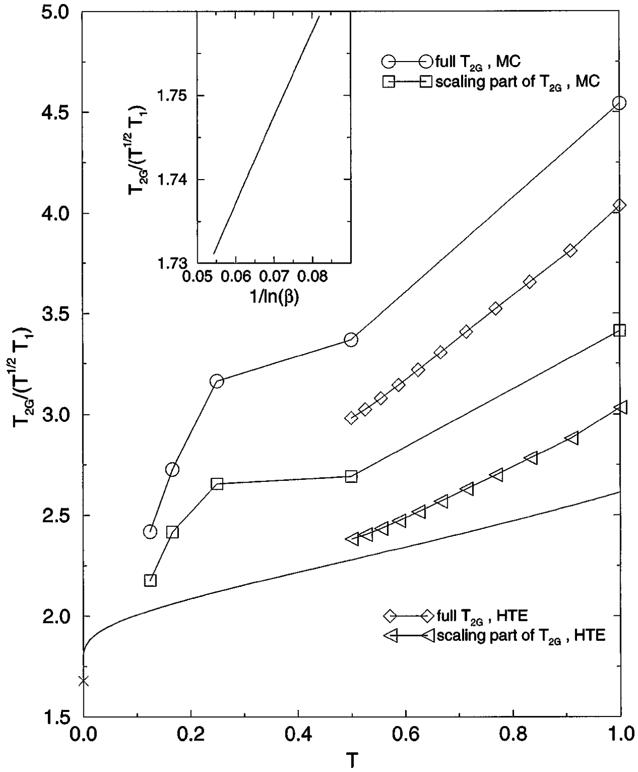

FIG. 3. The ratio $T_{2G}/\sqrt{T}\,T_1$ versus T from Eqs. (8) and (9). The $T = 0$ limit of the ratio is 1.68. The inset shows a linear variation with $1/\ln(\beta)$. QMC and HTE data for the ratio with full T_{2G} and with only the scaling part included are shown by the symbols.

$$\frac{1}{T_{2G}} = \frac{2^{-3+2\Delta}A_\perp^2(\pi)D}{\pi c}\,\sin(2\pi\Delta)\Gamma^2(1-2\Delta)I_2(\Delta) \times \sqrt{\frac{c}{T}\ln\frac{T_0}{T}}\,. \tag{9}$$

Here the integrals $I_1(\Delta) = \int_0^\infty dx\, \frac{x}{(\sinh x)^{4\Delta}}$ and $I_2^2(\Delta) = 4\int_0^\infty |\frac{\Gamma(\Delta - ix)}{\Gamma(1-\Delta-ix)}|^4$ have weak temperature dependences. In deriving Eq. (9), we have kept only the scaling part and dropped the term $[\sim\chi^2(x=0,\omega=0)]$ compensating on-site self interactions as it is down by a factor $T(\ln\frac{T_0}{T})^2$ and is beyond the limits of the scaling theory. We find that Eq. (8) shows weaker than $\sqrt{\ln(T_0/T)}$ variations with T. This result is in qualitative agreement with the recent measurement of $1/T_1$ in Sr_2CuO_3 by Takigawa *et al.* [3]. Figure 3 shows the ratio $T_{2G}/\sqrt{T}\,T_1$. In the $T \to 0$ limit our expressions (8) and (9) coincide with those of Sachdev [15]. However, we find that the $T = 0$ limit of $T_{2G}/\sqrt{T}\,T_1$ is approached with infinite slope, similar to the behavior of the uniform susceptibility [16]. The behavior is consistent with the slow rise of this quantity seen for Sr_2CuO_3 around $T = J/10$ [3].

Numerical results for χ'' are obtained from QMC data using the maximum-entropy (max-ent) method [19], and from HTE via the recursion method [17]. In Fig. 3, data are presented for the ratio with the full T_{2G} and with only the scaling part [where $\sim\chi^2(x=0,\omega=0)$ term is not subtracted] [20]. The two should converge in the scaling limit, and the *latter* should be compared with the theory. We found that QMC and HTE results for T_{2G} agree completely; deviations arise from the analytic continuation needed to get $1/T_1$, which is more uncertain for QMC data [21]. The difference between the curves based on the full T_{2G} and the scaling part 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 nonasymptotic contributions in the full T_{2G} and the apparent tendency of QMC + max-ent to slightly overestimate $1/T_1$ explain the discrepancy in the numerical result previously reported for $T_{2G}/\sqrt{T}\,T_1$ [21,22].

We also note that the experimental $1/T_1$ was found to be about 30% lower than the numerical result at $T = 300$ K [3,22], which is now also largely reconciled by more accurate QMC + max-ent results [21]. Considering also the good agreement found previously for $1/T_2$, without adjustable parameters [3,22], the spin-half chain indeed very well describes the low-frequency dynamics of Sr_2CuO_3.

The frequency-dependent quantities also do not show universality in the scaled variable ω/T. For example, the imaginary part of the local susceptibility

$[\chi(\omega) = \int_{-\infty}^{\infty} \frac{dq}{2\pi}\, \chi(q, \omega)]$ is given by

$$\chi''(\omega) = \frac{2^{2\Delta - 1/2} D}{c} \sin(2\pi\Delta) \left(\ln \frac{T_0}{T} \right)^{1/2} \Gamma(1 - 4\Delta) \times \left(\frac{\Gamma(2\Delta - i\, \frac{\omega}{2\pi T})}{\Gamma(1 - 2\Delta - i\, \frac{\omega}{2\pi T})} - \mathrm{H.c.} \right). \quad (10)$$

However, in the $T \to 0$ limit, it factorizes into a product of a nonuniversal amplitude and a universal function [4] of ω/T, $(\ln \frac{T_0}{T})^{1/2} \times \frac{\pi D}{c} \tanh(\frac{\omega}{2T})$.

QMC + max-ent data and theoretical results for $\chi''(0, \omega)$ are compared in Fig. 4, 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 ω/T. The numerical data are not at low enough temperatures to explore the scaling forms at larger ω/T. It would be useful to compare our results with neutron scattering data [23].

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_2CuO_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 ω/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 [24].

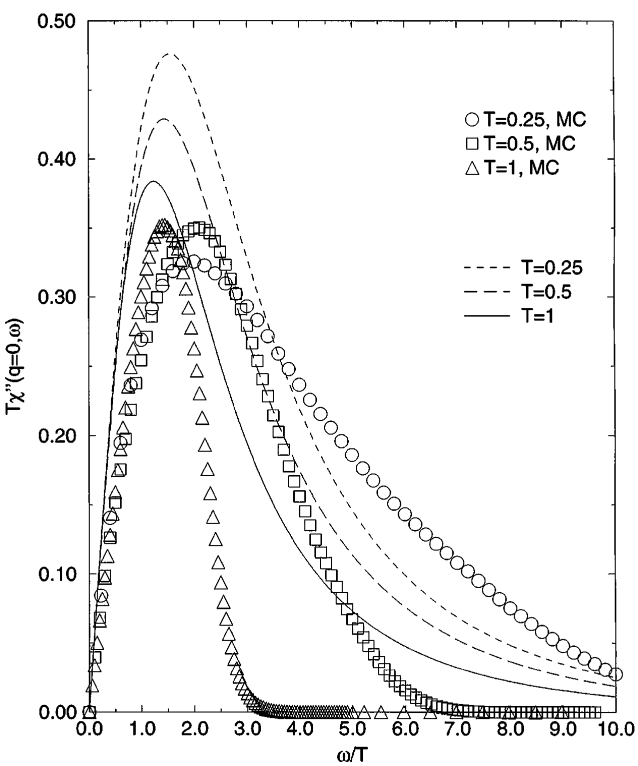

FIG. 4. Imaginary part of the antiferromagnetic susceptibility. Lines represent theoretical results with parameters as in Fig. 2, and the symbols represent the QMC + max-ent data.

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