Numerical evidence for multiplicative logarithmic corrections from marginal operators

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Field theory calculations predict multiplicative logarithmic corrections to correlation functions from marginally irrelevant operators. However, for the numerically most suitable model, the spin-$\frac{1}{2}$ chain, these corrections have been controversial. In this paper, the spin-spin correlation function of the antiferromagnetic spin-$\frac{1}{2}$ chain is calculated numerically in the presence of a next-nearest-neighbor coupling J_2 for chains of up to 32 sites. By varying the coupling strength J_2 we can control the effect of the marginal operator, and our results unambiguously confirm the field theory predictions. The critical value at which the marginal operator vanishes has been determined to be at $J_2/J = 0.241167 \pm 0.000005$. [S0163-1829(96)52538-5]

The spin-$\frac{1}{2}$ chain has attracted much attention in theoretical physics since the early days of quantum mechanics as a simple model for many-body effects. However, correlation functions in the antiferromagnetic chain could only be predicted with the help of field theory calculations,[1] and it was only a few years ago when a prediction of a *multiplicative* logarithmic correction to the asymptotic spin-spin correlation functions was made coming from a marginally irrelevant operator in the field theory description.[2,3] At first sight this result seems surprising, since it indicates that the effect of a marginally irrelevant operator effectively *increases* in the long-distance limit, while on the other hand, its effect on other quantities (energy spectrum,[2] susceptibility[4]) vanishes as length $L \rightarrow \infty$ and temperature $T \rightarrow 0$.

However, the underlying calculation which predicted the multiplicative correction from a marginal operator is quite general[5] and of great importance in other models as well (e.g., the ϕ^4 model). Since the spin-$\frac{1}{2}$ chain is accessible by a number of numerical methods, it represents an ideal testing model for this important result. Therefore, considerable effort has been made to verify the logarithmic corrections,[6–8] but often different or no multiplicative corrections were found.

In the present paper we choose to numerically diagonalize the model Hamiltonian of up to 32 sites exactly. While this method is limited by relatively small system sizes, it allows us to introduce a next-nearest neighbor coupling J_2 quite easily and, moreover, the results are very accurate. It is known that by adjusting J_2 we can change the bare coupling strength of the marginal operator and even set it to zero without destroying the validity of the field theory continuum limit.[9] Since we are able to probe the system with a reduced marginal coupling, the range of validity for the perturbative field theory calculations is increased exponentially. Moreover, we will use an approach to analyze the data which does not depend on any extrapolation to an infinite system size for the field theory calculations to be valid, so that 32 sites turn out to be very sufficient to confirm the effect unambiguously.

Our model Hamiltonian is the antiferromagnetic spin-$\frac{1}{2}$ chain ($J>0$) with a next-nearest neighbor coupling J_2

$$H = J\sum_x \mathbf{S}_x \cdot \mathbf{S}_{x+1} + J_2 \sum_x \mathbf{S}_x \cdot \mathbf{S}_{x+2}. \tag{1}$$

In the long-wavelength, low-energy limit this model is well understood in terms of the Wess-Zumino-Witten (WZW) nonlinear σ model with a topological coupling constant $k=1$.[10] In the continuum limit, the spin-$\frac{1}{2}$ operator $\mathbf{S}_x$ at each lattice site x can then be expressed in terms of a WZW SU(2) matrix g_α^β and (related) chiral SU(2) currents $\mathbf{J}_{L,R}$

$$\mathbf{S}_x = (\mathbf{J}_L + \mathbf{J}_R) + \text{const } i(-1)^x \text{tr}[g\boldsymbol{\sigma}]. \tag{2}$$

Strictly speaking this theory is only valid up to correcting higher-order operators in the Hamiltonian which we have neglected so far. In particular, we want to consider the effect of the leading irrelevant marginal operator which can be written in terms of the current operators with some coupling constant λ

$$\delta\mathcal{H} = -2\pi\lambda \mathbf{J}_L \cdot \mathbf{J}_R. \tag{3}$$

For periodic boundary condition the next ''leading'' irrelevant operator in the Hamiltonian has scaling dimension 4, which can be neglected even for modest lengths of order $L \gtrsim 10$ and temperatures of order $T \lesssim 0.1J$[11]

The effect of the marginal operator on the uniform (i.e., current-current) part of the spin-spin correlation function is well understood in terms of a simple additive logarithmic correction. This leads to interesting predictions for the asymptotic behavior of the susceptibility,[4] which were well confirmed by Bethe ansatz and also experimental results.[12] The situation is quite different, however, for the alternating part of the spin-spin correlation function $G(r)$ which is given in terms of the WZW field g

$$G(r) \propto \langle \text{tr}[g\boldsymbol{\sigma}](0)\text{tr}[g\boldsymbol{\sigma}](r)\rangle. \tag{4}$$

For the primary field g we have to take into account the effect of the marginal operator on the anomalous scaling dimension $\gamma(\lambda)$ of tr$[g\boldsymbol{\sigma}]$ as well (while the scaling dimension of the currents is fixed). The correlation function then also depends on the marginal coupling constant λ, and $G(r,\lambda)$ obeys the renormalization equation

$$\left(\frac{\partial}{\partial \ln r} + \beta(\lambda)\frac{\partial}{\partial\lambda} + 2\gamma(\lambda)\right) G(r,\lambda) = 0, \tag{5}$$

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TABLE I. The spin-spin correlation function $\langle S_z(0)S_z(r)\rangle$ for various values of $r=L/2$ and J_2. In some cases the last digit is uncertain.

$r=L/2$	$J_2=-0.25J$	$J_2=0$	$J_2=0.1J$	$J_2=0.2J$	$J_2=J_2^{\mathrm{crit}}$
4	0.0572167	0.0497077	0.0459760	0.0417541	0.0398672
5	-0.0545609	-0.0469513	-0.0433261	-0.0390852	-0.0370562
6	0.0423313	0.0356626	0.0325190	0.0288716	0.0271334
7	-0.0403820	-0.0340938	-0.0311410	-0.0276488	-0.0259367
8	0.0336161	0.0279325	0.0252780	0.0221537	0.0206302
9	-0.0322537	-0.0269130	-0.0244137	-0.0214326	-0.0199523
10	0.0279427	0.0230233	0.0207281	0.0179995	0.0166504
11	-0.0269492	-0.0223039	-0.0201300	-0.0175197	-0.0162116
12	0.0239555	0.0196206	0.0175960	0.0151709	0.0139598
13	-0.0232004	-0.0190837	-0.0171551	-0.0148271	-0.0136519
14	0.0209966	0.0171185	0.0153044	0.0131186	0.0120183
15	-0.0204030	-0.0167013	-0.0149649	-0.0128595	-0.0117902
16	0.0187105	0.0151987	0.0135530	0.0115605	0.0105511

where $\beta(\lambda)$ is the beta function of the marginal operator $\delta\mathcal{H}$. Equation (5) is then solved by introducing a scale dependent coupling constant $\lambda(r)$ which obeys

$$\frac{\partial\lambda}{\partial \ln r}=\beta(\lambda) \tag{6}$$

and writing (up to a prefactor which may contain additive corrections in λ)

$$G(r)\propto \exp\left(-2\int_{\ln r_1}^{\ln r}\gamma(x)d(\ln x)\right)$$
$$=\exp\left(-2\int_{\lambda_0}^{\lambda(r)}\frac{\gamma(\lambda)}{\beta(\lambda)}d\lambda\right), \tag{7}$$

where r_1 is an ultraviolet cut-off of the order of the lattice spacing and λ_0 is the unrenormalized (bare) coupling strength at that energy scale. The beta function and the anomalous dimension are known as perturbative expansions in λ (Ref. 2)

$$\beta(\lambda)=-\lambda^2+\mathcal{O}(\lambda^3),$$
$$\gamma(\lambda)=\frac{1}{2}-\frac{\lambda}{4}+\mathcal{O}(\lambda^2). \tag{8}$$

Integrating Eq. (6), we obtain an expression for λ up to $\mathcal{O}[\ln(\ln r)/(\ln r)^2]$

$$\lambda(r)\approx\frac{\lambda_0}{1+\lambda_0\ln(r/r_1)}=\frac{1}{\ln(r/r_0)}, \tag{9}$$

and together with Eq. (7) we can determine the correlation function up to higher orders in λ

$$G(r)\propto\frac{(\lambda/\lambda_0)^{-1/2}}{r}[1+\mathcal{O}(\lambda)]\approx\frac{\sqrt{\lambda_0\ln r/r_0}}{r}. \tag{10}$$

From Eq. (9) we see that the constant r_0 is simply given by

$$r_0=r_1\exp(-1/\lambda_0). \tag{11}$$

In the asymptotic limit we find $G\propto\sqrt{\ln r}/r$ as already predicted in Ref. 2 unless λ_0 is infinitesimally small. Therefore, very close to the critical point the predicted asymptotic limit will never be reached although the perturbative expansions in Eq. (8) are very accurate. Since r_0 is a nonuniversal constant, it is essential to keep the full expression in Eq. (10) to test that result (as opposed to just assuming the asymptotic limit).

It is important to note that Eq. (5) is only valid if r is the only length scale in the system, but all previous studies assumed that this would require the infinite length limit $L\rightarrow\infty$ which is numerically very difficult to achieve. However, it is perfectly feasible to study the system at finite, but varying lengths L and keeping the ratio $R=r/L$ fixed. Since $r=RL$ is no longer independent of L, there is only one variable parameter in the problem and therefore expression (10) holds for $G(r=RL)$ (for each R separately, i.e., the overall proportionality constant will depend on the choice of R). To test the field theory predictions it is therefore much easier and more accurate to select the fixed ratio to be $R=\frac{1}{2}$, and in what follows we will hence set

$$r\equiv L/2. \tag{12}$$

It is then straightforward to determine the correlation function $G(r=L/2)$ numerically for different lengths $L\leqslant 32$ and coupling constants J_2 (as opposed to selecting $R=0$ and having to choose some controversial[6,7] extrapolation to the $L\rightarrow\infty$ limit as in all previous studies).

The correlation functions of the ground state were found by exact diagonalization using the modified Lanczos method on periodic spin chains of up to 32 sites (using ca. 4.7 million basis states). Table I shows the results for the spin-spin correlation functions $\langle S_z(0)S_z(r)\rangle$ for different distances $r=L/2$ and for various values of the next-nearest-neighbor coupling J_2.

By adjusting J_2 we can change the bare coupling λ_0 and even set it to zero at some critical value J_2^{crit}.[9] To lowest order, λ_0 increases linearly with the difference from the critical point $\Delta J_2\equiv J_2^{\mathrm{crit}}-J_2$. The critical value J_2^{crit} was determined to be

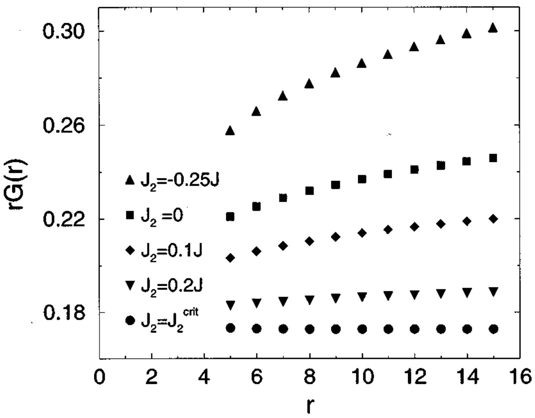

FIG. 1. The multiplicative correction $rG(r)$ as a function of r for various values of J_2 according to the numerical data in Table I.

$$J_2^{\text{crit}} \approx 0.241167 \pm 0.000005 J, \tag{13}$$

which we believe to be the most accurate estimate to date. This result was obtained by examining the energy difference Δ between the first two excited states of total spin $S=0$ and $S=1$ in the periodic chain spectrum as a function of length L and J_2. Those two states are nearly degenerate and their energy difference is only due to the marginal operator and higher-order terms in the field theory Hamiltonian. We find the critical point by determining the value of J_2 at which the energy difference Δ is exactly proportional to $1/L^3$, because at that point the correction Δ comes only from the higher-order terms and therefore the marginal operator is absent.[11] This approach proves to be more accurate than the conventional method of extrapolating the value of $J_2(\Delta=0)$ as $L \to \infty$ (which, of course gives the same value, although with less accuracy[13]).

As we approach J_2^{crit} the value of the effective length scale r_0 becomes exponentially small $r_0 = r_1 \exp(-1/\lambda_0)$, and the expansions in $1/\ln(r/r_0)$ in Eqs. (9) and (10) give very accurate results even for moderate lengths. However, we require the marginal operator to remain the *leading* correction (compared to the $1/L^2$ corrections from higher-order operators), so it is not always useful to examine the system arbitrarily close to J_2^{crit}.

To extract the multiplicative correction we perform a cubic spline interpolation of $r\langle S_z(0) S_z(r)\rangle$ from the data in Table I for even and odd r separately. The difference between the two curves then gives the multiplicative correction $rG(r)$ to the alternating part of the correlation function as shown in Fig. 1 for different values of J_2.

Figure 2 shows the excellent asymptotic fit to the predicted form of the multiplicative corrections

$$rG(r) = \sqrt{a\lambda_0 \ln r/r_0} \tag{14}$$

with the fitting parameters given in Table II where a is a normalization constant which must be independent of λ_0. In all cases the data approaches the asymptotic curve very quickly. The small deviations are positive for small values of $\Delta J_2 \equiv J_2^{\text{crit}} - J_2$ and negative for larger ΔJ_2, which indicates a partial cancellation of higher-order terms with varying relative magnitude as λ_0 is changed (this explains why the first-order calculation already gives such good results).

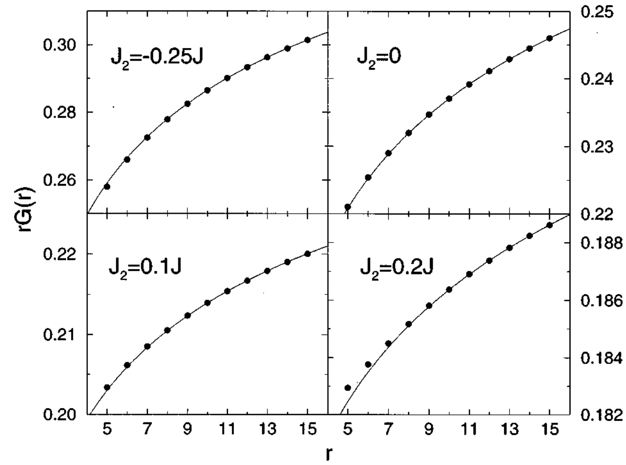

FIG. 2. The fitting curves to $rG(r)$ according to Eq. (14) with the parameters given in Table II.

For the special $J_2=0$ case we find general agreement with Ref. 6 where a similar fit was made, however with much larger deviations, and, more importantly, their data does not approach the predicted form asymptotically as it must. (In that reference an extrapolation scheme with additional adjustable parameters was used as well as a less accurate numerical method.)

As the critical point is approached, we require simultaneously $r_0 \to 0$ and $\lambda_0 \to 0$ in such a way that the correlation function $G(r)$ remains finite. In particular we know from Eq. (11) that r_0 and λ_0 are related [to lowest order the correlation function $G(r)$ is independent of the size of the marginal coupling at the ultraviolet cutoff r_1] i.e., for all $J_2 \leq J_2^{\text{crit}}$ we must have

$$\lambda_0 \ln(r_1/r_0) = 1. \tag{15}$$

As can be seen in Fig. 3 this relation holds very accurately for the parameters in Table II for all values of J_2 with the constant in Eq. (14) given by $a=0.0296$. Equation (15) also fixes the ultraviolet cutoff $r_1=0.85$ at which the bare coupling constant is defined. Because a and r_1 are fixed, λ_0 and r_0 are related by Eq. (15), and there remains really only one free parameter for each of the curves in Fig. 2, which makes the quality of the fits even more impressive.

TABLE II. The fitting parameters according to Eq. (14) for selected values of J_2.

J_2/J	$\ln r_0$	$a\lambda_0$
-0.25	-1.4976	0.021601
-0.1	-2.1683	0.014864
0	-2.9501	0.010696
0.05	-3.6111	0.008626
0.1	-4.6883	0.006546
0.15	-6.9080	0.004383
0.2	-14.393	0.002080

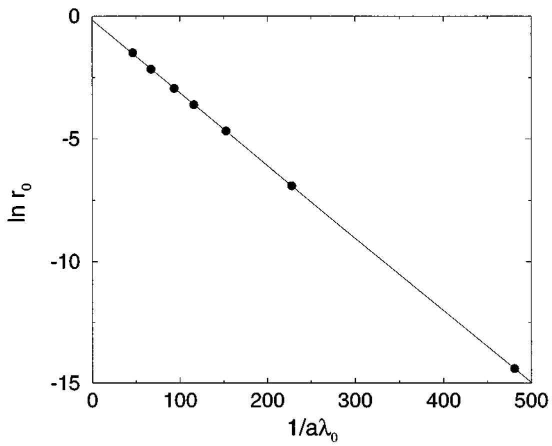

FIG. 3. The logarithm $\ln r_0$ vs $1/a\lambda_0$ from Table II shows an excellent fit to $\ln r_0 = \ln r_1 - 1/\lambda_0$ with $r_1 = 0.85$ and $a = 0.0296$, confirming Eq. (15).

Moreover, analyzing the fitting parameters in Table II, we can determine the functional behavior of the bare coupling λ_0 in form of a series expansion in the microscopic parameter $\Delta J_2 = J_2^{\text{crit}} - J_2$

$$\lambda_0 = c_1 \Delta J_2 + c_2 \Delta J_2^2 + c_3 \Delta J_2^3. \tag{16}$$

As shown in Fig. 4, this relation (16) seems to hold even for relatively large values of ΔJ with $c_1 \approx 1.723/J$, $c_2 \approx -1.35/J^2$, and $c_3 \approx 1.76/J^3$. Therefore, once the constants a, r_1, and c_i are known, the shape and overall magnitude of $G(r)$ can be predicted accurately for a large range of values J_2 and $r \gtrsim 5$, which is a clear success of the field theory calculation.

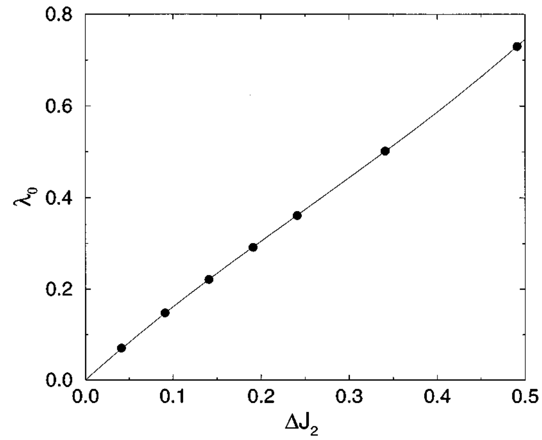

FIG. 4. The parameter λ_0 vs $\Delta J_2 \equiv J_2^{\text{crit}} - J_2$ from Table II is fitted to Eq. (16).

In conclusion, we have unambiguously shown that the field theory calculations for multiplicative corrections to the correlation functions in the spin-$\frac{1}{2}$ chain are valid. The constants a, r_1, and c_i were determined, and we were able to improve the estimate of J_2^{crit}. The basic result carries over to other models with marginal operators (one-dimensional Hubbard model, other half-integer spin chains, ϕ^4 models) where we also expect that the corresponding field theory calculation gives accurate predictions to multiplicative corrections to correlation functions.

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