Numerical Evidence for Multiplicative Logarithmic Corrections from Marginal Operators

Sebastian Eggert

Theoretical Physics, Chalmers University of Technology and Göteborg University, 41296 Göteborg, Sweden
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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-1/2 chain – these corrections have been controversial. In this paper, the spin-spin correlation function of the antiferromagnetic spin-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 \( J_2/J = 0.241167 \pm 0.000005 \).

The spin-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 \[4\], 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 \[\phi^4\]. 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 \[\phi^4\], susceptibility \[\phi^4\]) vanishes as length \( L \to \infty \) and temperature \( T \to 0 \).

However, the underlying calculation which predicted the multiplicative correction from a marginal operator is quite general \[\phi^4\] and of great importance in other models as well (e.g. the \( \phi^4 \)-model). Since the spin-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 \[\phi^4\], 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 \[\phi^4\]. 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 a novel 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-1/2 chain \((J > 0)\) with a next nearest neighbor coupling \( J_2 \)

\[
H = J \sum_x S_x \cdot S_{x+1} + J_2 \sum_x S_x \cdot S_{x+2}.
\]  (1)

In the long-wavelength, low-energy limit this model is well understood in terms of the Wess-Zumino-Witten (WZW) non-linear \( \sigma \)-model with a topological coupling constant \( k = 1 \). In the continuum limit, the spin-1/2 operator \( S_x \) at each lattice site \( x \) can then be expressed in terms of a WZW SU(2) matrix \( g_\beta \) and (related) chiral SU(2) currents \( J_{L,R} \)

\[
S_x = (J_L + J_R) + \text{const.} i(-1)^x \text{tr}[g_{\beta}].
\]  (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 \( \lambda \)

\[
\delta H = -2\pi \lambda J_L \cdot J_R.
\]  (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 \( T \lesssim 0.1J \).

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 \[ \lambda_0 \], which were well confirmed by Bethe ansatz and also experimental results [13]. 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 \[ g \]

\[ G(r) \propto < \text{tr}[g \sigma(0)] \cdot \text{tr}[g \sigma(r)] > . \]  

(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 \[ \text{tr}[g \sigma] \] as well (while the scaling dimension of the currents is fixed). The correlation function then also depends on the marginal coupling constant \( \lambda \), and \[ G(r, \lambda) \] obeys the renormalization equation

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

(5)

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

\[ \frac{\partial \lambda}{\partial \ln r} = \beta(\lambda) \]  

(6)

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

\[ G(r) \propto \exp \left[ -2 \int_{\ln r_1}^{\ln r} \gamma(x) d(\ln x) \right] \]

\[ = \exp \left[ -2 \int_{\lambda_0}^{\lambda(r)} \frac{\gamma(\lambda)}{\beta(\lambda)} d\lambda \right], \]  

(7)

where \( r_1 \) is an ultraviolet cut-off of the order of the lattice spacing and \( \lambda_0 \) is the unrenormalized (bare) coupling strength at that energy-scale. The beta-function and the anomalous dimension are known as perturbative expansions in \( \lambda \)

\[ \beta(\lambda) = -\lambda^2 + \mathcal{O}(\lambda^3) \]

\[ \gamma(\lambda) = \frac{1}{2} - \frac{\lambda}{4} + \mathcal{O}(\lambda^2). \]  

(8)

Integrating equation (8), we obtain an expression for \( \lambda \) up to \( \mathcal{O}[\ln(\ln r)/\ln r] \)

\[ \lambda(r) \approx \frac{\lambda_0}{1 + \lambda_0 \ln(r/r_1)} = \frac{1}{\ln(r/r_0)}, \]  

(9)

and together with equation (5) we can determine the correlation function up to higher orders in \( \lambda \)

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

(10)

From equation (5) we see that the constant \( r_0 \) is simply given by

\[ r_0 = r_1 \exp(-1/\lambda_0), \]  

(11)

In the asymptotic limit we find \( G \propto \sqrt{\ln r}/r \) as already predicted in reference [3] unless \( \lambda_0 \) is infinitesimally small. Therefore, very close to the critical point the predicted asymptotic limit will never be reached although the perturbative expansions in equation (5) are very accurate. Since \( r_0 \) is a non-universal constant, it is essential to keep the full expression in equation (10) to test that result (as opposed to just assuming the asymptotic limit).

It is important to note that equation (8) 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 \( L \to \infty \) 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 \( R = 1/2 \), and in what follows we will hence set

\[ r \equiv L/2. \]  

(12)

It is then straightforward to determine the correlation function \( G(r = L/2) \) numerically for different lengths \( L \leq 32 \) and coupling constants \( J_2 \) (as opposed to selecting \( R = 0 \) and having to choose some controversial extrapolation to the \( L \to \infty \) 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 \( \lambda_0 \) and even set it to zero at some critical value \( J_2^{\text{crit}} \). To lowest order, \( \lambda_0 \) increases linearly with the difference from the critical point \( \Delta J_2 \equiv J_2^{\text{crit}} - J_2 \). The critical value \( J_2^{\text{crit}} \) was determined to be

\[ J_2^{\text{crit}} \approx 0.241167 \pm 0.000005 J, \]  

(13)

which we believe to be the most accurate estimate to date. This result was obtained by examining the energy difference \( \Delta \) 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 $\Delta$ is exactly proportional to $1/L^3$, because at that point the correction $\Delta$ comes only from the higher order terms and therefore the marginal operator is absent \cite{2}. 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 \cite{4}).

As we approach $J_2^{\text{crit}}$ 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 equations (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 $J_2^{\text{crit}}$.

To extract the multiplicative correction we perform a cubic spline interpolation of $r < S_z(0)S_z(r) >$ 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 figure (1) for different values of $J_2$.

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

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

with the fitting parameters given in table II where $a$ is a normalization constant which must be independent of $\lambda_0$. In all cases the data approaches the asymptotic curve very quickly. The small deviations are positive for small values of $\Delta J_2 = J_2^{\text{crit}} - J_2$ and negative for larger $\Delta J_2$, which indicates a partial cancellation of higher order terms with varying relative magnitude as $\lambda_0$ is changed (this explains why the

| $r = L/2$ | $J_2 = -0.25J$ | $J_2 = 0$ | $J_2 = 0.1J$ | $J_2 = 0.2J$ | $J_2 = J_2^{\text{crit}}$ |
|-----------|----------------|-----------|--------------|--------------|---------------------|
| 4         | 0.0572167      | 0.0497077 | 0.0459760    | 0.0417541    | 0.0398672           |
| 5         | -0.0545609     | -0.0469513| -0.043261    | -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| -0.024437    | -0.0214326   | -0.0199523          |
| 10        | 0.0279427      | 0.0220233 | 0.0207281    | 0.0179995    | 0.0166504           |
| 11        | -0.0269492     | -0.0210837| -0.017551    | -0.0148271   | -0.0136519          |
| 12        | 0.0239555      | 0.0186206 | 0.0175960    | 0.0157099    | 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   | -0.0128505   | -0.0117902          |
| 16        | 0.0187105      | 0.0151987 | 0.0135530    | 0.0117506    | 0.0105511           |

TABLE I. The spin-spin correlation function $< S_z(0)S_z(r) >$ for various values of $r = L/2$ and $J_2$. In some cases the last digit is uncertain.
At which the bare coupling constant is defined. Because $a$ and $r_1$ are fixed, $\lambda_0$ and $r_0$ are related by equation (13), and there remains really only one free parameter for each of the curves in figure (3), which makes the quality of the fits even more impressive.

| $J_2/J$ | $\ln r_0$ | $a\lambda_0$ |
|--------|-----------|-------------|
| -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    |

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

For the special $J_2 = 0$ case we find general agreement with reference [7] 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 equation (11) that $r_0$ and $\lambda_0$ 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:

$$\lambda_0 \ln \frac{r_1}{r_0} = 1$$

(15)

As can be seen in figure (3) this relation holds very accurately for the parameters in table I for all values of $J_2$ with the constant in equation (14) given by $a = 0.0296$. Equation (13) also fixes the ultraviolet cutoff $r_1 = 0.85$.
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[1] E-mail address: eggert@fy.chalmers.se
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