Logarithmic corrections of one-dimensional $S = \frac{1}{2}$ Heisenberg antiferromagnet

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We investigate the effect of the marginal operator on the critical exponents of the one-dimensional $S = \frac{1}{2}$ Heisenberg model, using the relation between the critical exponents and the energy gaps of the finite system. The energy gaps behave as $\Delta E \propto 1/L$ with the logarithmic corrections from the marginally irrelevant operator. The numerical results obtained with the Bethe ansatz are well explained by the two-loop renormalization of the marginal coupling. Thus the discrepancies between the one-loop renormalization prediction and numerical results are resolved, though it is found that the nonuniversal constant of the logarithmic correction in the ground state does not agree with the asymptotic expansion of the Bethe ansatz.

The one-dimensional Heisenberg model

$$H = \sum_{i=1}^{L} \mathbf{S}_i \cdot \mathbf{S}_{i+1} \tag{1}$$

is one of the simplest many-body problems but shows several nontrivial behaviors. It is discussed that half-odd-integer spin Heisenberg models belong to the same universality class as the S=1/2 case,[1] and so it is important to understand the S=1/2 Heisenberg model more deeply.

The various properties of the S=1/2 Heisenberg model are well understood. The energy eigenvalue problem is solved using the Bethe ansatz. Unfortunately, the spin correlation cannot be calculated with the Bethe ansatz. The critical exponent η of the spin correlation $\langle \mathbf{S}_0 \cdot \mathbf{S}_r \rangle \propto (-1)^r r^{-\eta}$ has been obtained as $\eta = 1$ indirectly by bosonization.[2] However, results of exact diagonalization are somewhat different from this value.[3] It was pointed out that the umklapp process produces a logarithmic correction,[4,5] and this term makes the convergence of the finite-size correction extremely slow.

Another approach to investigate the correlation function is to use conformal field theory.[6] The critical exponent is related to the energy gap of the finite-size system with periodic boundary conditions,[7]

$$E_n(L) - E_0(L) = 2\pi v x/L, \qquad 2x = \eta. \tag{2}$$

The other important formula is the finite-size correction of the ground state energy[8]

$$E_0(L) = e_0 L - \pi v c/6L, \tag{3}$$

where c is the conformal anomaly number that plays a central role in conformal field theory. In (2),(3) v is the "sound velocity" for the model [in this case $v = \pi/2$ (Ref. 9)]. The finite-size corrections of the ground state energy and the energy gaps of the S=1/2 spin chain can be obtained with the Bethe ansatz, and these results indicate that $c = 1$ (Refs. 10 and 11) and $x = 1/2$.[12] Although for $c < 1$ the assumption of conformal invariance and unitarity yields a discrete set of possible value of c and critical exponents, there are no constraints on c and critical exponents for $c \geq 1$. Nonetheless if the system has an internal non-Abelian symmetry, such as SU(2) of the spin chain, there are other restrictions on the critical indices (Kac-Moody algebra).[13] In our case, the S=1/2 Heisenberg antiferromagnet corresponds to the SU(2) Wess-Zumino-Witten (WZW) model with topological coupling $k = 1$.

In addition to relevant operators, in the WZW model there is a marginal operator $\mathbf{J}_L \cdot \mathbf{J}_R$, which causes logarithmic corrections on the energy gap, the spin-correlation function, and other quantities.[14] However, it is found that there are some discrepancies between the one-loop renormalization prediction and the numerical results obtained with the Bethe ansatz for the finite system.[14] In our previous paper, we noticed the importance of the two-loop correction.[15] We consider in this paper the two-loop renormalization of the marginal operator more deeply.

Conformal invariance is exact only at the fixed point. In general there exist irrelevant operators, which produce finite-size corrections vanishing more rapidly than $1/L$. We can calculate the correction terms if we know the operator product expansion (OPE) of irrelevant operators and other primary fields at the fixed point. Let us consider a critical Hamiltonian as

$$H = H^* + g \int d^2x \phi(x), \tag{4}$$

where H^* is a fixed point Hamiltonian and ϕ is an irrelevant operator whose scaling dimension is x. Mapping this onto a cylinder and carrying out the first-order perturbation, we obtain[16]

$$E_n(L) - E_0(L) = \frac{2\pi}{L} \left[x_n + 2\pi b_n g \left(\frac{2\pi}{L} \right)^{x-2} \right] \tag{5}$$

(for simplicity we set $v = 1$). Under a change of length scale, the coupling g satisfies the renormalization equation[17]

$$\beta(g) \equiv dg/dl = (2 - x)g - \pi b g^2 + O(g^3). \tag{6}$$

The OPE coefficients b, b_n are related to the normalizations of the three-point functions of ϕ, ϕ_n,[18] and the ratios of them are universal.

When ϕ is marginally irrelevant, that is, $x = 2$ and $bg(l) > 0$, the solution for (6) is

$$\pi b g(l) = \pi b g_0/(1 + \pi b g_0 l) = 1/(\ln L + 1/\pi b g_0), \tag{7}$$

where we set $e^l = L$. Substituting this into (5), we see that

$$E_n(L) - E_0(L) = \frac{2\pi}{L}\left(x_n + \frac{2b_n}{b}\frac{1}{\ln(L/L_0)}\right). \tag{8}$$

For the SU(2) $k = 1$ WZW model, the scaling dimensions of the lowest triplet and singlet excitations are $x_t = x_s = 1/2$. In this case, the coefficients b_n, b are easily obtained by the OPE of the currents $\mathbf{J}_L, \mathbf{J}_R$ and other primary fields in the Kac-Moody algebra. These are $b_t/b = -1/8$ for the triplet excitation and $b_s/b = 3/8$ for the singlet excitation.[14]

In Eq. (6), we treat the β function up to $O(g^2)$, and we obtain the $O(1/\ln L)$ correction. If we consider the β function up to $O(g^3)$, there appears an $O(\ln(\ln L)/(\ln L)^2)$ term, which cannot be negligible until L becomes very large. Since higher-order terms than $O(g^3)$ depend on regularization, we neglect these terms.[19,20] Consider the next equation

$$dg/dl = -\pi b g^2 - \pi^2 d g^3, \tag{9}$$

and integrate this; we obtain

$$\ln(L/L_0) = 1/\pi b g - (d/b^2)\ln(1/\pi b g + d/b^2). \tag{10}$$

For $L \gg 1$, this is approximated as

$$\pi b g \approx \frac{1}{\ln(L/L_0)} - \frac{d}{b^2}\frac{\ln[\ln(L/L_0) + d/b^2]}{\ln^2(L/L_0)}. \tag{11}$$

It is shown that the SU(2) $k = 1$ WZW model is equivalent to the sine-Gordon model at $\beta^2 = 8\pi$.[21] From the two-loop β function of the sine-Gordon equation, the constants b, d of Eq. (9) satisfy $d/b^2 = 1/2$.[20] The two-loop β functions for the general WZW models can be deduced from those of the chiral Gross-Neveu models,[22] which have been proven to be equivalent to the WZW models.[21]

Another important effect of the marginal coupling is a correction of $O(g^3)$ to the ground state energy,[17]

$$E_0(L) = e_0 L - (\pi/6L)[c + (8/b^2)(\pi b g)^3]. \tag{12}$$

Thus the correction from a marginal operator to the ground state energy converges much faster than those of energy gaps. Note that although ratios of b, b_n are universal, the number b itself depends on normalization of ϕ.

The eigenvalues of the Heisenberg Hamiltonian (1) are given by the following Bethe ansatz equations:

$$\left(\frac{\lambda_j - i/2}{\lambda_j + i/2}\right)^L = -\prod_{k=1}^{M}\left(\frac{\lambda_j - \lambda_k - i}{\lambda_j - \lambda_k + i}\right), \quad j = 1, \ldots, M, \tag{13}$$

where M is related to the total spin S as $S = L/2 - M$. From these roots $\{\lambda_j\}$, the energy eigenvalues are given by

$$E = \frac{L}{4} - \sum_{j=1}^{M}\frac{2}{4\lambda_j^2 + 1}. \tag{14}$$

The ground state has $L/2$ real λ, the lowest triplet state has $L/2-1$ real λ, and the singlet excited state has $L/2-2$ real λ plus a complex pair at $\pm i/2$.

Applying the Euler-Maclaurin formula and a Wiener-Hopf integration to (13), Woynarovich and Eckle,[23] Avdeev and Dörfel,[24] and Hamer *et al.*[25] obtain analytically the asymptotic behaviors of the ground state energy, the triplet excitation, and the singlet excitation. Their results are consistent with those of conformal field theory taking account of the marginal operator up to the one-loop order.

Unfortunately, there are still no analytic results up to the two-loop order.[27] So we solve the Bethe ansatz equations (13) numerically and compare these results with the predictions of conformal field theory with the marginal operator up to the two-loop order.

Numerical Bethe ansatz results were obtained for the ground state energy and the lowest triplet and singlet excited states energy by Avdeev[26] up to $L = 480$ and Affleck *et al.*[14] up to $L = 2048$. We calculate these energy eigenvalues up to $L = 16384$.[28] These results are shown in Table I. In order to extract the critical exponents and finite-size corrections by irrelevant operators, we use the following notations in this table:

$$\begin{aligned} c(L) &= (6L/\pi v)[e_0 L - E_0(L)], \\ x_t(L) &= (L/2\pi v)[E_t(L) - E_0(L)], \\ x_s(L) &= (L/2\pi v)[E_s(L) - E_0(L)]. \end{aligned} \tag{15}$$

In the large limit($L \to \infty$), these values become $c = 1$ and $x_t = x_s = 1/2$, but convergences are extremely slow.

We investigate the effect of the marginal operator from these data. Several authors[15,23,25] have noticed that the $O(\ln[\ln(L)]/[\ln(L)]^2)$ term in (11) is important to interpret numerical data. In this paper we will use Eq. (10) directly. First we consider the triplet excitation. From Eq. (8), we obtain

$$\pi b g_t(L) \equiv 4[\tfrac{1}{2} - x_t(L)] \simeq \pi b g(L), \tag{16}$$

where $\pi b g(L)$ is defined by (10). Analyzing our data for L=1024–16384 based on this form, we obtain $L_0 = 0.5653(2)$. In Fig. 1 we compare the effective coupling

TABLE I. Numerical Bethe ansatz results. $c(L)$, $x_t(L)$, and $x_s(L)$ are defined in Eq. (15).

L	$c(L)$	$x_t(L)$	$x_s(L)$
256	1.0010323251382	0.46483064034411	0.62048957293961
320	1.0009288547119	0.46598413601509	0.61611034218623
384	1.0008553503974	0.46686952717954	0.61276252507011
512	1.0007556014624	0.46817285465041	0.60785771757117
640	1.000689395739	0.4691125952419	0.6043396084766
768	1.000641274677	0.4698386771392	0.6016325407402
1024	1.000574490607	0.4709150256942	0.5976382879858
1280	1.000529206963	0.4716966703695	0.5947521988068
1536	1.000495806787	0.4723037914637	0.5925192144511
2048	1.00044876532	0.473208906275	0.589204710787
2560	1.00041640617	0.473870027515	0.586794911158
3072	1.00039229458	0.474385755907	0.584921763161
4096	1.00035797509	0.475158223449	0.582127270984
5120	1.00033411561	0.475725181338	0.580084852983
6144	1.0003161996	0.47616905245	0.57849099708
8192	1.0002904886	0.47683651084	0.57610288561
10240	1.0002724630	0.47732839655	0.57434963108
12288	1.0002588428	0.47771467578	0.57297679508
16384	1.0002391643	0.47829748719	0.57091218791

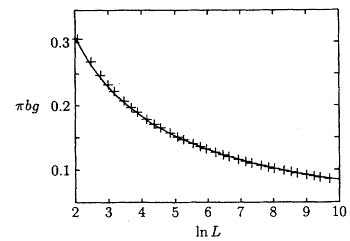

FIG. 1. Comparison of the effective coupling constant $g_t(+)$ and the two-loop renormalized coupling (solid line).

$\pi b g_t$ and the two-loop renormalization prediction (10). In the whole region the agreement of both is good. This indicates that there is no $O(g^2)$ or higher correction.

Next we consider the singlet excitation. In Fig. 2 we plot the g_s/g_t as a function of $\pi b g_t$, where $\pi b g_s$ is defined as

$$\pi b g_s(L) \equiv \tfrac{4}{3}[x_s(L) - \tfrac{1}{2}]. \tag{17}$$

Figure 2 indicates that the marginal correction of the singlet excitation contains not only the $O(g)$ term, but also an $O(g^2)$ term. These results are represented as

$$\begin{aligned} \pi b g_s(L) &= c_1 \pi b g_t(L) + c_2[\pi b g_t(L)]^2, \\ c_1 &= 1.00065(6), \quad c_2 = 1.0198(7), \end{aligned} \tag{18}$$

Perhaps both c_1 and c_2 may be a universal value 1.

As for the finite-size correction of the ground state energy, to extract the coefficient of the $(\pi bg)^3$ term, we plot $[c(L)-1]/(\pi b g_t)^3$ as a function of $\pi b g_t \simeq 1/\ln(L)$ in Fig. 3(a). The coefficient of $(\pi bg)^3$ approaches a constant 0.365 and there is no $O(g^4)$ term. About the irrelevant operator, there is an $O(L^{-2})$ correction which comes from the operator $L_{-2}\bar{L}_{-2}\mathbf{1}$ (Ref. 17) [see Fig. 3(b)]. The amplitude of $O(L^{-2})$ is large since it occurs in first order, while other irrelevant operators occur in second order. These results are represented as

$$\begin{aligned} c(L) &= 1 + c_3\,(\pi b g(L))^3 + c_4 L^{-2}, \\ c_3 &= 0.36516(2), \\ c_4 &= 1.66(6). \end{aligned} \tag{19}$$

Our fit 0.365 for the coefficient of $(\ln L)^{-3}$ agrees neither with 0.3433 by Woynarovich and Eckle[23] nor 3/8 by Affleck *et al.*[14] An explanation of the contradiction is the dropping of higher-order terms of the Euler-Maclaurin formula which is used to replace a sum with an integral[26] (also see Appendix). These higher terms change the values of the largest root Λ and root density $\sigma_L(\Lambda), \sigma'_L(\Lambda)$, etc. As for the universal constants corresponding to $x_n, 2b_n/b$ in (8), the effects of $\Lambda, \sigma_L(\Lambda), \ldots$ are canceled out, but in the case of the nonuniversal constant corresponding to b in (12), it is necessary to take account of the variation of $\Lambda, \sigma_L(\Lambda), \ldots$.

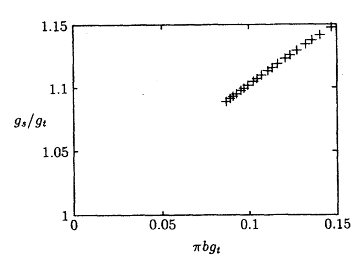

FIG. 2. g_s/g_t as a function of the $\pi b g_t$. This indicates that g_s has an $O(g^2)$ correction besides g.

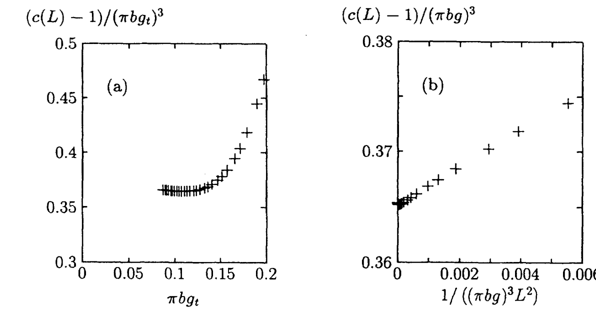

FIG. 3. (a) $(c(L)-1)/(\pi b g_t)^3$ as a function of the $\pi b g_t$. It seems that the coefficient of $(\pi bg)^3$ approaches a constant 0.365. (b) $(c(L)-1)/(\pi bg)^3$ as a function of the $1/((\pi bg)^3 L^2)$. This indicates that $c(L)$ has an $O(L^{-2})$ correction besides $O(g^3)$.

Finally we consider the spin-correlation function. The Green function $G_n(r) \equiv \langle \phi_n(r)\phi_n(0)\rangle$ obeys a renormalization group equation

$$[r(\partial/\partial r) + \beta(g)(\partial/\partial g) + 2\gamma_n(g)]G_n = 0. \tag{20}$$

The regularization independent parts of $\beta(g)$ and $\gamma_n(g)$ are[14,19]

$$\beta(g) = -\pi b g^2 - \pi^2 d g^3, \quad \gamma_n(g) = x_n + 2\pi b_n g. \tag{21}$$

Using these relations, we obtain

$$G_n(r,g) = G_n(r_0)\exp\left[-\int_{r_0}^{r} \frac{dr'}{r'} 2\gamma_n\right] = C\mathcal{G}_n(r), \tag{22}$$

where

$$\begin{aligned} \mathcal{G}_n(r) &= r^{-2x_n}[1/\pi b g(r) + d/b^2]^{-4b_n/b}, \\ C &= G(r_0)/\mathcal{G}_n(r_0). \end{aligned} \tag{23}$$

The spin-correlation function is proportional with the

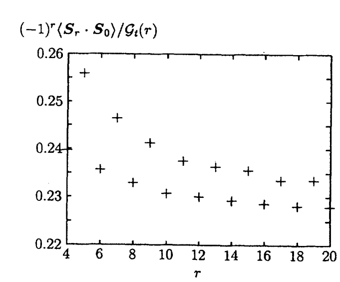

FIG. 4. $(-1)^r\langle \mathbf{S}_r \cdot \mathbf{S}_0\rangle/\mathcal{G}_t(r)$ as a function of r. The correlation functions $\langle \mathbf{S}_r \cdot \mathbf{S}_0\rangle$ are Monte Carlo data by Kubo *et al.* (Ref. 29).

Green function

$$\langle \mathbf{S}_r \cdot \mathbf{S}_0 \rangle \propto (-1)^r G_t(r) + \mathrm{const}/r^2, \tag{24}$$

where $x_t = 1/2$ and $b_t/b = -1/8$. In Fig. 4, we compare $\mathcal{G}_t(r)$ with the Monte Carlo data by Kubo *et al.*[29] Although the length of chain is rather small, the agreement of two results is pretty well. Remaining corrections seem to be of power-law type.

Kubo *et al.* concluded that $\langle \mathbf{S}_r \cdot \mathbf{S}_0 \rangle \propto (-1)^r (\ln r)^{0.25}/r$ from their data, which contradicts the one-loop renormalization prediction $(-1)^r (\ln r)^{0.5}/r$.[5] By taking account of the renormalization up to the two-loop order, this discrepancy is cleared up.

In conclusion, the two-loop renormalization of the marginal coupling well explains the numerical Bethe ansatz results. It is expected to calculate the L_0 of Eq. (11) by the analytic Bethe ansatz and to reexamine the derivation of the nonuniversal coefficient of $(\ln L)^{-3}$ in the ground state energy.

We would like to thank Professor I. Affleck for pointing out Destri's paper on the two-loop β function of the Gross-Neveu model. We also thank Professor M. Takahashi, Dr. K. Ishida, Dr. K. Okamoto, and Dr. T. Koma for fruitful discussions. Most parts of our calculation were done on the NEC EWS4800/220 workstation.

APPENDIX

When λ_j are all real, (13) is rewritten as $L\phi(\lambda_j) = 2\pi I_j + \sum_{k=1}^{m} \phi((\lambda_j - \lambda_k)/2)$, where $\phi(\lambda) \equiv 2\arctan(2\lambda)$, and the I_j are integers or half-integers. Following Woynarovich and Eckle,[23] we define a function $z_L(\lambda) = (1/2\pi)[\phi(\lambda) - (1/L)\sum_{j=1}^{m} \phi((\lambda - \lambda_j)/2)]$ and its derivative $\sigma_L(\lambda) = dz_L(\lambda)/d\lambda$, so that $z_L(\lambda_j) = I_j/L$. We also define the inverse function of $z_L(\lambda)$ as $\lambda(z_L)$. One can use the Euler-Maclaurin formula to show that

$$\frac{1}{L}\sum g(\lambda_j) = \int_{-\lambda(z_m)}^{\lambda(z_m)} g(\lambda(z))dz + \frac{1}{2L}[g(\lambda(z_m)) + g(\lambda(-z_m))] + \frac{1}{12L^2}\left[\frac{d}{dz}g(\lambda(z))\bigg|_{z_m} - \frac{d}{dz}g(\lambda(z))\bigg|_{-z_m}\right]$$
$$-\frac{1}{720L^4}\left[\frac{d^3}{dz^3}g(\lambda(z))\bigg|_{z_m} - \frac{d^3}{dz^3}g(\lambda(z))\bigg|_{-z_m}\right] + \text{higher terms.}$$

In the third term the magnitude of the parenthesis is $(d/dz)g(\lambda(z))|_{z_m} = [1/\sigma_L(\Lambda)]g(\Lambda)$, and in the fourth term

$$\frac{d^3}{dz^3}g(\lambda(z))\bigg|_{z_m} = 3\frac{\sigma_L'(\Lambda)^2}{\sigma_L(\Lambda)^5}g'(\Lambda) - \frac{\sigma_L''(\Lambda)}{\sigma_L(\Lambda)^4}g'(\Lambda) - 3\frac{\sigma_L'(\Lambda)}{\sigma_L(\Lambda)^4}g''(\Lambda) + \frac{1}{\sigma_L(\Lambda)^3}g'''(\Lambda),$$

where $\Lambda = \lambda(z_m)$. Considering that $\sigma_L(\Lambda), \sigma_L'(\Lambda), \sigma_L''(\Lambda)$ are $O(1/L)$, the contributions of the third, fourth, and higher terms are $O(1/L)$.

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