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1997 J. Phys. A: Math. Gen. 30 6287

(http://iopscience.iop.org/0305-4470/30/18/012)

J. Phys. A: Math. Gen. **30** (1997) 6287–6298. Printed in the UK PII: S0305-4470(97)82956-3

Critical properties of the spin-$\frac{1}{2}$ Heisenberg chain with frustration and bond alternation

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Received 1 April 1997

Abstract. We study the $S = \frac{1}{2}$ Heisenberg chain with frustration and alternation which is expressed by $\mathcal{H} = \sum_j \{[1 + (-1)^j \delta] \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1} + J_2 \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+2}\}$, both analytically and numerically. We focus on the $J_2 = 0.2411$ case, where there is no marginal operator which brings about the logarithmic corrections in various quantities. By using the bosonization method, we calculate the energy gap, the change in the ground-state energy due to the alternation (so-called energy gain), the spin correlation and the string correlation (not only their exponents but also their amplitudes), and compare them with the results of the numerical diagonalization for finite systems. We point out the existence of the logarithmic correction in the energy gain despite the absence of the marginal operator. Taking into account this logarithmic correction, we can obtain a reasonable hyperscaling relation between the critical exponents of the energy gap and an energy gain from the numerical data.

1. Introduction

Recently, the ground-state phase transitions due to the quantum effects in low-dimensional systems have attracted much attention. Let us consider the isotropic $S = \frac{1}{2}$ Heisenberg chain with next-nearest-neighbour interactions expressed by

$$\mathcal{H}_0 = \sum_{j=1}^{N} \{\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1} + J_2 \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+2}\} \tag{1.1}$$

which is one of the simplest models of the spin system with frustrations. When $J_2 = 0$, the ground state of (1.1) is the spin-fluid state [1], which is characterized by the gapless excitation and the algebraic decay of the spin correlations. When $J_2 = \frac{1}{2}$, on the other hand, Majumdar and Ghosh [2] and Majumdar [3] found that the direct products of the local singlet dimers

$$\begin{aligned} &\Psi_1 = [1, 2][3, 4] \cdots [N-1, N] \qquad \Psi_2 = [2, 3][4, 5] \cdots [N, 1] \\ &[i, j] \equiv \frac{1}{\sqrt{2}} \left(\uparrow_i \downarrow_j - \downarrow_i \uparrow_j\right) \end{aligned} \tag{1.2}$$

are the ground state of (1.1) in case of even N and the periodic boundary condition. Therefore the ground-state phase transition from the spin-fluid state to the doubly degenerate

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0305-4470/97/186287+12$19.50

dimer (DDD) state is expected to be between $J_2 = 0$ and $J_2 = \frac{1}{2}$ [4]. Okamoto and Nomura (ON) [5–7] studied this fluid-dimer transition by the numerical diagonalization of the finite-size Hamiltonian with the help of the bosonization, renormalization group method, conformal field theory, and the physical insight into how the doubly degenerate state is realized in infinite systems. They concluded that the critical value J_{2c} of the fluid-dimer transition is

$$J_{2c} = 0.2411 \tag{1.3}$$

from the numerical diagonalization data up to 24 spins. They also studied the critical properties. Their value was confirmed by Castilla *et al* [8], and Eggert [9].

We can write down the effective Hamiltonian [4–6, 10] for (1.1) after the bosonization as

$$\mathcal{H}_{0b} = \int \mathrm{d}x \, \{A(\nabla\theta)^2 + C P^2 + D\cos 2\theta\} \tag{1.4}$$

where $[\theta(x), P(x')] = \mathrm{i}\delta(x - x')$ and the detailed expressions for the coefficients A, C and D are shown in section 2. In the spin-fluid region, the term $\cos 2\theta$ is marginal, which brings about the logarithmic corrections in various physical quantities [5–7]. In the dimer region, on the other hand, this term is relevant, which results in the gapful excitation and the dimer long-range order. ON manifested that this fluid-dimer transition is of the Berezinskii–Kosterlitz–Thouless type and $D = 0$ at J_{2c}. Therefore, at J_{2c}, the effective Hamiltonian (1.4) is purely Gaussian and the logarithmic corrections vanish. We note that J_{2c} and the Gaussian point do not coincide for the fluid-dimer transition of the models with XY-like anisotropy, as explained in [6].

Let us introduce the bond alternation

$$\mathcal{H}_1 = \delta \sum_j (-1)^{j+1} \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1} \qquad \delta > 0 \tag{1.5}$$

to system (1.1). When $J_2 \leqslant J_{2c}$, $\mathcal{H}_1$ yields the change in the ground state from the spin-fluid state to the dimer state. This dimer state is unique (we call it the UD state). For $J_2 > J_{2c}$, the DDD state is resolved by $\mathcal{H}_1$ and the ground state is the UD state. The phase diagram of the system $\mathcal{H}_0 + \mathcal{H}_1$ is shown in figure 1. The state Ψ_1 is the true ground state on the line $\delta + 2J_2 = 1$, as shown by Shastry and Sutherland [11].

When $J \leqslant J_{2c}$, the critical behaviour of the second-order phase transition can be observed as $\delta \to 0$. Let us define the energy gap exponent ν by

$$\Delta E(\delta) \sim \delta^{\nu} \qquad \delta \to 0 \tag{1.6}$$

and the energy gain exponent a by

$$G(\delta) \equiv E_0(0) - E_0(\delta) \sim \delta^{a} \tag{1.7}$$

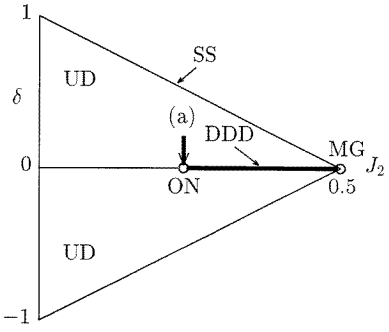

Figure 1. The ground-state phase diagram of $\mathcal{H}_0 + \mathcal{H}_1$. The Majumdar–Ghosh point ($\delta = 0$, $J_2 = 0.5$) is denoted by MG. The ON point ($\delta = 0$, $J_2 = 0.2411$) is the fluid-dimer transition point determined by Okamoto and Nomura. The DDD state is realized on the line between ON and MG points. UD means the unique dimer state. Ψ_1 (Ψ_2) is the unique ground state on the SS line $\delta + 2J_2 = 1$ ($-\delta + 2J_2 = 1$). In this paper we consider the critical behaviour along the line (a).

where $E_0(\delta)$ is the ground-state energy. These values were analytically calculated as $\nu = \frac{2}{3}$ and $a = \frac{4}{3}$ by Cross and Fisher [12], and Nakano and Fukuyama [13] for the $J_2 = 0$ case. Because these values can be related to the $SU(2)$ symmetry of the Hamiltonian, they still hold even for the system $\mathcal{H}_0 + \mathcal{H}_1$ when $0 \leqslant J_2 \leqslant J_{2c}$. Black and Emery [14], however, pointed out $\Delta E(\delta) \sim \delta^{2/3}/\sqrt{|\log \delta|}$, of which logarithmic correction comes from the marginal term $D\cos 2\theta$ in (1.4). This logarithmic correction explains the fact that the exponent ν obtained from the numerical diagonalization (for the $J_2 = 0$ case) was somewhat larger than the predicted value $\frac{2}{3}$ [15, 16]. If the logarithmic correction is taken into account in the analysis of the numerical data, the calculated critical exponent ν becomes nearer to $\frac{2}{3}$ [17].

At J_{2c}, the above-mentioned logarithmic correction vanishes because $D = 0$. Thus, the pure power-law behaviour may be observed in $\Delta E(\delta)$ as $\delta \to 0$. Chitra, Pati, Krishnamurthy, Sen and Ramasesha (CPKSR) [18] performed the density matrix renormalization group calculation for $\mathcal{H}_0+\mathcal{H}_1$ at $J_{2c} = 0.2411$ to conclude $\nu = 0.667\pm0.001$ and $a = 1.251 \pm 0.001$. Although their value of ν agreed with $\frac{2}{3}$ very well, that of a was slightly smaller than the predicted value $\frac{4}{3}$. If we map the present one-dimensional quantum system onto the two-dimensional classical system, the energy gain corresponds to the anomalous part of the free energy associated with the phase transition. Thus, the exponent a is translated into $2-\alpha$ in the language of the two-dimensional classical system, where α is the exponent of the specific heat. The well known hyperscaling relation

$$d\nu = 2 - \alpha \tag{1.8}$$

means

$$2\nu = a \tag{1.9}$$

in the present quantum one-dimensional notation. Therefore the result of CPKSR violates the hyperscaling relation, although they did not seem to recognize it. Then we believe that it is worthwhile making a careful investigation on the various critical behaviours of the system $\mathcal{H}_0 + \mathcal{H}_1$ at J_{2c}.

We note that the system $\mathcal{H}_0 + \mathcal{H}_1$ is not only interesting from the standpoint of the statistical physics, but also important to recognize the properties of existing materials. In fact, an inorganic spin-Peierls compound $CuGeO_3$ is thought to be well modelled by $\mathcal{H}_0+\mathcal{H}_1$ with $\delta = 0.03$ [8] and $J_2 = 0.24 \sim 0.36$ [8, 19].

This paper is organized as follows. We summarize the analytical prediction on the critical behaviours of the energy gap, the energy gain, the Néel correlation and the string correlation by using the bosonized Hamiltonian in section 2. We compare the numerical results of the exact diagonalization with the analytical predictions in section 3. Finally, section 4 is devoted to discussion.

2. Analytical predictions

Let us begin with the XXZ version of the model described in section 1 for convenience

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 \tag{2.1}$$

$$\mathcal{H}_0 = \sum_j \{(\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1})_\Delta + J_2(\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+2})_\Delta\} \tag{2.2}$$

$$\mathcal{H}_1 = \delta \sum_j (-1)^{j+1}(\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1})_\Delta \qquad \delta > 0 \tag{2.3}$$

where

$$(\boldsymbol{S}_i \cdot \boldsymbol{S}_j)_\Delta \equiv S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z. \tag{2.4}$$

The bosonized Hamiltonian of (2.2) is of the sine-Gordon form [7]

$$\mathcal{H}_{0b} = \int \mathrm{d}x \, \{A(\nabla\theta)^2 + C P^2 + D\cos 2\theta\} \tag{2.5}$$

where $[\theta(x), P(x')] = \mathrm{i}\delta(x - x')$ and the coefficients are

$$\begin{aligned} A &= \frac{1}{8\pi}\left(1 + \frac{3\Delta}{\pi} + \frac{(6+\Delta)J_2}{\pi}\right) \\ C &= 2\pi\left(1 - \frac{\Delta}{\pi} - \frac{(2-\Delta)J_2}{\pi}\right) \\ D &= \frac{\Delta - (2+\Delta)J_2}{2}. \end{aligned} \tag{2.6}$$

We take the spin spacing as the unit length. Since these expressions for A, C and D are reliable only near $\Delta = 0$ and $J_2 = 0$, we cannot correctly obtain J_{2c} itself from the bosonized Hamiltonian (2.5). It is widely believed, however, that the critical properties are well described by the bosonized Hamiltonian.

The renormalization group equations for the sine-Gordon Hamiltonian (2.5) up to the lowest order are

$$\frac{\mathrm{d}y_0(l)}{\mathrm{d}l} = -y_\theta^2(l) \qquad \frac{\mathrm{d}y_\theta(l)}{\mathrm{d}l} = -y_\theta(l)y_0(l) \tag{2.7}$$

where $y_0(0)$ and $y_\theta(0)$ are defined by

$$y_0(0) \equiv \frac{g_0}{\pi v_s} \qquad y_\theta(0) \equiv \frac{g_\theta}{\pi v_s} \tag{2.8}$$

with

$$K \equiv \frac{1}{2\pi}\sqrt{\frac{C}{A}} \equiv 1 + \frac{g_0}{2\pi v_s} \qquad g_\theta \equiv 2\pi^2 D \qquad v_s \equiv 2\sqrt{AC}. \tag{2.9}$$

In the spin-fluid region ($J \leqslant J_{2c}$), the long-distance asymptotic behaviours of the spin correlations are governed by the quantity K as

$$\langle S_i^z S_j^z\rangle \sim |i-j|^{-K} \qquad \langle S_i^+ S_j^-\rangle \sim |i-j|^{-1/K} \tag{2.10}$$

except for the logarithmic corrections, and v_s is the spin wave velocity. The flow diagram of (2.7) is shown in figure 2. Let us consider the $\Delta = 1$ case, on which we will focus. When $\Delta = 1$ and $J \leqslant J_{2c}$, the quantity K should be renormalized to 1 because two spin correlations of (2.10) exhibit the same behaviour due to the symmetry. Therefore the starting point of the renormalization, $(y_0(0), y_\theta(0))$, lies on the fluid-Néel boundary line as far as $J_2 < J_{2c}$. As J_2 increases from 0, the point $(y_0(0), y_\theta(0))$ moves on this line towards the origin where the fluid-dimer transition occurs. Thus $y_\theta(0) = 0$ (i.e. $D = 0$) at J_{2c}, which means that the sine-Gordon Hamiltonian is reduced to Gaussian. The logarithmic corrections in various physical quantities vanish at J_{2c}, since they are originated from the marginal term $D\cos 2\theta$ in (2.5). We note that the Gaussian point ($y_\theta(0) = 0$ or $D = 0$) and the fluid-dimer transition point do not coincide for the XY-like case ($\Delta < 1$), as explained in [6].

The bosonized expression of the bond alternation term is [20, 21]

$$\mathcal{H}_{1b} = -\int \mathrm{d}x \left\{\delta\cos\theta + \frac{\delta\Delta}{\pi}(\nabla\theta)^2\cos\theta\right\}. \tag{2.11}$$

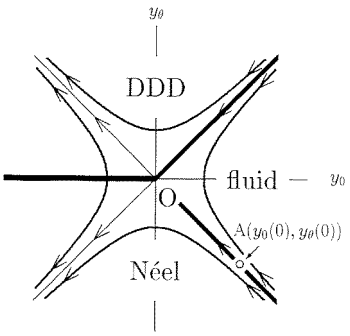

Figure 2. The flow diagram of the renormalization equations (2.7) on the y_0–y_θ plane. The phase boundaries are shown by heavy lines. When $\Delta = 1$, the starting point of the renormalization, A$(y_0(0), y_\phi(0))$, lies on the fluid-Néel boundary as far as $J_2 < J_{2c}$.

The $\delta \cos\theta$ term comes from the x and y components of the bond alternation and the $(\delta\Delta/\pi)(\nabla\theta)^2 \cos\theta$ term from the z component.

Since we focus on the $\Delta = 1$ and $J_2 = J_{2c}$ case, our bosonized Hamiltonian is

$$\mathcal{H}_b = \int dx \left\{ \frac{v_s}{4\pi}(\nabla\theta)^2 + \pi v_s P^2 - \delta\cos\theta - \frac{\delta}{\pi}(\nabla\theta)^2\cos\theta \right\} \tag{2.12}$$

where we have used $K = 1$. Since the expressions of A and C in (2.6) are not exact in the quantitative sense as already stated, it is not appropriate to use the value of v_s derived from $v_s = 2\sqrt{AC}$ with (2.6). Therefore we treat v_s as a parameter for a while and later substitute the numerically calculated data.

Although the renormalization group method is powerful, it is essentially the theory of the logarithmic accuracy. Because we want to analytically obtain not only the critical exponents of various physical quantities but also their amplitudes to compare with the numerical results, we apply the self-consistent harmonic approximation (SCHA) which is essentially the variational method. We choose the trial Hamiltonian of the SCHA as

$$\mathcal{H}_{SCHA} = \int dx \left\{ \frac{v_s}{4\pi}(\nabla\theta)^2 + \pi v_s P^2 + \tilde{B}\theta^2 \right\}. \tag{2.13}$$

Here $\tilde{B}$ is the variational parameter which should be determined by

$$\frac{\partial \langle \mathcal{H}_b \rangle_{SCHA}}{\partial \tilde{B}} = 0 \tag{2.14}$$

where $\langle \cdots \rangle_{SCHA}$ denotes the average with respect to the ground state of $\mathcal{H}_{SCHA}$.

Since the SCHA calculation for $\mathcal{H}_b$ in (2.12) is described in [13, 21, 22], we summarize the SCHA results without going into details. The excitation spectrum is

$$\omega(q) = v_s\sqrt{q^2 + q_c^2} \tag{2.15}$$

where q_c is determined by the self-consistent equation

$$\frac{v_s q_c^2}{4\pi} = \frac{3\delta}{4}\sqrt{\frac{q_c}{2\pi}} \tag{2.16}$$

which results in

$$q_c = \left(\frac{9\pi}{2v_s^2}\right)^{1/3} \delta^{2/3}. \tag{2.17}$$

We note that the first factor on the r.h.s. of (2.17) slightly depends on the method to cut off the short wavelength contribution. The energy gap of the finite system is

$$\Delta E(\delta, N) = \omega\left(\frac{\pi}{N}\right) = v_s\sqrt{\left(\frac{\pi}{N}\right)^2 + q_c^2}. \tag{2.18}$$

This equation is reduced to formula (3.3) based on the conformal field theory.

The Néel correlation function is expressed as [22]

$$\mathcal{O}_{\rm Neel}(j-l) \equiv \langle S_j^z S_l^z \rangle = A_{\rm Neel}\delta^{2/3}\sinh\{K_0(q_c|j-l|)\} \tag{2.19}$$

where $K_0(x)$ is the zeroth-order modified Bessel function of the second kind and $A_{\rm Neel}$ is a constant which depends on the short wavelength cut-off. Using the asymptotic behaviour of $K_0(x)$

$$K_0(x) \simeq \sqrt{\frac{\pi}{2x}}\,{\rm e}^{-x} \qquad (x \to \infty) \tag{2.20}$$

we can see the exponential decay of $\mathcal{O}_{\rm Neel}(j-l)$ as expected. The physical quantity which characterizes the UD state is the string correlation $\mathcal{O}_{\rm UD}(j-l)$ defined by [23]

$$\mathcal{O}_{\rm UD}(j-l) \equiv -4\langle S_j^z \exp\{{\rm i}\pi(S_j^{z+1} + S_{j+2}^z + \cdots + S_{l-1}^z)S_l^z\}\rangle \tag{2.21}$$

where j and l are odd integers. According to [23], $\mathcal{O}_{\rm UD}(j-l)$ is calculated as

$$\mathcal{O}_{\rm UD}(j-l) = A_{\rm UD}\delta^{1/6}\exp[K_0(q_c|j-l|)/4] \tag{2.22}$$

where $A_{\rm UD}$ is a cut-off-dependent constant. The long-range order value of $\mathcal{O}_{\rm UD}(j-l)$ as $|j-l| \to \infty$ is

$$\mathcal{O}_{\rm UD}(\infty) = A_{\rm UD}\delta^{1/6}. \tag{2.23}$$

3. Numerical results

We performed the numerical diagonalization of finite systems up to $N = 26$ spins under the periodic boundary condition to find the energies and the Néel and string correlations of the ground and low-lying excited states.

First we discuss the spin wave velocity v_s for $\delta = 0$ case, which is necessary to compare the numerical and analytical results quantitatively. Since the system is in the spin fluid state when $\delta = 0$, we can obtain the spin wave velocity from the finite-size correction of the ground-state energy of the N-spin system with the help of the conformal field theory [24, 25]

$$E_0(0, N) = N\epsilon_0(0, \infty) - \frac{\pi c v_s}{6N} + {\rm O}(N^{-3}) \tag{3.1}$$

where $\epsilon_0(\delta, N)$ is the ground-state energy per spin, and c is the conformal charge which is unity in our problem. The ${\rm O}(N^{-3})$ correction comes from the irrelevant operators which are not included in the sine-Gordon scheme [7]. We note that there is no $\log N$ correction in (3.1) because the marginal operator vanishes at J_{c2}. Analysing the ground-state energy data by using (3.1) (see figure 3), we obtain

$$v_s = 1.174. \tag{3.2}$$

Another method to determine v_s is to use the formula [26]

$$\Delta E(N) = \frac{\pi v_s K}{N} + {\rm O}(N^{-3}) \tag{3.3}$$

where $\Delta E(N)$ is the energy gap for the N-spin system and $K = 1$ in the present case as was explained in section 2. The origin of ${\rm O}(N^{-3})$ is the same as that in (3.1). The spin wave velocity obtained from the energy gap data (see figure 4) is $v_s = 1.174$, which shows very good agreement with (3.2).

From (2.18), the finite-size energy gap is written as the finite-size scaling form [27]

$$\delta^{-2/3}\Delta E(\delta, N) = f_{\rm gap}(N\delta^{2/3}) \tag{3.4}$$

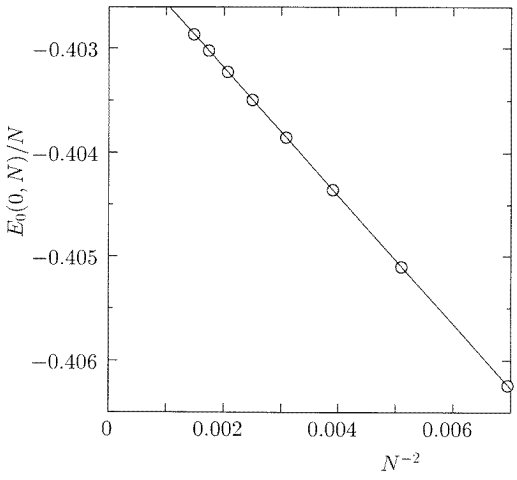

Figure 3. Plot of the ground-state energy per one spin as a function of N^{-2}. When we take only the first and second terms on the r.h.s. of equation (3.1), $E_0(0, N)/N = -0.401\,95–0.6173\,N^{-2}$ (full curve) gives the best fit, from which we obtain $v_s = 1.179$. If we take the N^{-4} (or higher) term into account, we obtain $v_s = 1.174$.

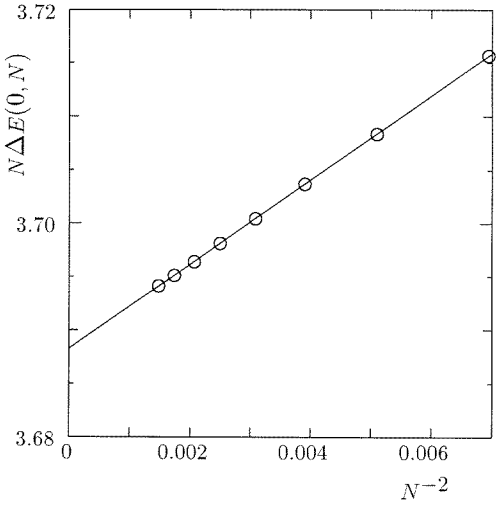

Figure 4. Plot of $N\Delta E(N)$ as a function of N^{-2}. The equation $N\Delta E(N) = 3.6883 + 3.9435\,N^{-2}$ (full curve) gives the best fit, which results in $v_s = 1.174$. When $O(N^{-4})$ correction is taken into account, the value $v_s = 1.174$ is unchanged.

where

$$f_{\text{gap}}(x) = v_s\sqrt{A_{\text{gap}}^2 + \pi^2 x^{-2}}. \tag{3.5}$$

Although we can easily see $A_{\text{gap}} = 2.173$ from equations (2.17), (2.18) and (3.2), it depends on how the short wavelength cut-off is introduced. Thus, we treat A_{gap} as a fitting parameter. Figure 5 shows the finite-size scaling plot of $\Delta E(\delta, N)$. All the points are on the universal curve, which strongly supports $\nu = \frac{2}{3}$. When we choose $\nu = 0.65$ or $\nu = 0.68$, we can clearly observe the scattering of the data points. From the horizontal part of the plot for larger $N\delta^{2/3}$ we see $v_s A_{\text{gap}} = 2.15$, i.e.

$$A_{\text{gap}} = 1.83. \tag{3.6}$$

The full line represents (3.5) with (3.6), which shows very good agreement with the numerical data.

The energy gain $G(\delta, N)$ for the finite system (N spins) is defined by

$$G(\delta, N) \equiv E_0(0, N) - E_0(\delta, N). \tag{3.7}$$

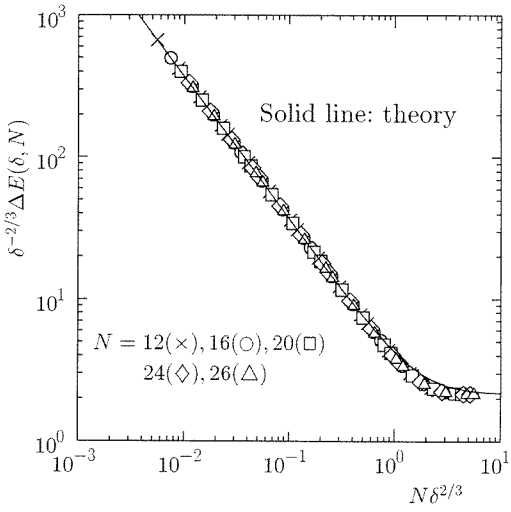

Figure 5. Finite-size scaling plot of $\Delta E(N)$. The fitting parameter $A_{\rm gap}$ in equation (3.5) can be determined from horizontal part of the plot.

The reduction of the numerical accuracy is severe for $G(\delta, N)$, as is easily seen from its definition (3.7). Therefore, instead of $G(\delta, N)$ itself, we use

$$\tilde{G}(\delta, N) \equiv \frac{\partial G(\delta, N)}{\partial \delta} = -\frac{\partial E_0(\delta, N)}{\partial \delta}$$
$$= -\left\langle \frac{\partial \mathcal{H}}{\partial \delta} \right\rangle = \frac{N}{2}(\langle \boldsymbol{S}_1 \cdot \boldsymbol{S}_2 - \boldsymbol{S}_2 \cdot \boldsymbol{S}_3 \rangle) \tag{3.8}$$

where the Feynman's relation is employed. Since $\tilde{G}(\delta, N) \sim \delta^{a-1}$, the finite-size scaling form of $\tilde{G}(\delta, N)$ is

$$\delta^{1-a}\tilde{G}(\delta, N) \sim \tilde{f}_{\rm gain}(N\delta^{2/3}). \tag{3.9}$$

Thus, we can determine the exponent a so that the data points of $\delta^{1-a}\tilde{G}(\delta, N)$ versus $N\delta^{2/3}$ are on the universal curve. The curves (b)–(d) show (3.9) with $a = \frac{4}{3}$, 1.29 and 1.25, respectively. As can be seen from figure 6, the universal fit is unsatisfactory. Namely, the best fit is observed by $a = 1.29$ for $N\delta^{2/3} < 10^{-1}$, whereas by $a = 1.25$ for $N\delta^{2/3} > 10^{0}$. Thus, unfortunately, we cannot accurately determine the exponent a. Further the hyperscaling relation $a = 2\nu$ is violated whether $a = 1.29$ or $a = 1.25$. We have tried the finite-size scaling plot for $G(\delta, N)$ itself for a check to find a similar phenomena.

The above-mentioned poor universality of the scaling plot suggests the existence of the contribution other than the algebraic one. As was stated in section 2, the logarithmic correction originated from the marginal term (i.e. $D\cos 2\theta$ term in (2.5)) is absent in our case. However, in the alternating XY chain without next-nearest-neighbour interaction ($\Delta = J_2 = 0$ in (2.1)–(2.3)), there exists a logarithmic correction in the energy gain $G(\delta)$ and not in the energy gap $\Delta E(\delta)$. Namely, the exact solution of this model [28] leads to $G(\delta) \sim \delta^2|\log\delta|$ and $\Delta E(\delta) \sim \delta$. If we suppose

$$G(\delta) \sim \delta^a|\log\delta| \tag{3.10}$$

the finite-size scaling form of $\tilde{G}(\delta, N)$ is

$$\frac{\delta^{1-a}}{1 + p|\log\delta|}\tilde{G}(\delta, N) = \tilde{g}_{\rm gain}(N\delta^{2/3}) \tag{3.11}$$

where p is a constant and $\tilde{g}_{\rm gain}(x)$ is a scaling function. We have plotted (3.11) with sweeping a and p, and found that the best universal plot is obtained by $a = \frac{4}{3}$ and $p = 0.11$

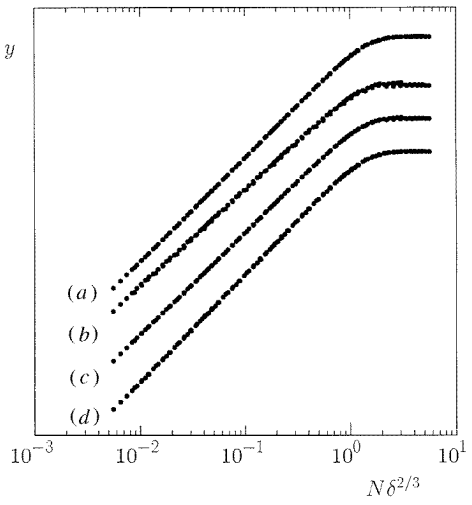

Figure 6. Finite-size scaling plot of $\tilde{G}(\delta)$. For (a) y represents (3.11) with $a = \frac{4}{3}$ and $p = 0.11$, and for (b)–(d) y represents (3.9) with $a = \frac{4}{3}, 1.29$ and 1.25, respectively. We have shifted each curve along the vertical axis for clarity. The plot (a) exhibits better universal fitting than the others.

on the whole region, as shown by figure 6(a). The plot (a) has better universality than the others. Thus the behaviour (3.10) with $a = \frac{4}{3}$ is quite plausible, although we cannot completely rule out the possibility of the pure power law behaviour. The origin of the logarithmic correction in $G(\delta)$ will be discussed in the next section.

Let us choose $j - l = N/2 = M$ for the Néel correlation of the N-spin system, because the periodic boundary condition is imposed. From (2.19) the finite-size scaling form of the Néel correlation is

$$M\mathcal{O}_{\text{Neel}}(\delta, M) = f_{\text{Neel}}(M\delta^{2/3}) \tag{3.12}$$

where

$$f_{\text{Neel}}(x) = A_{\text{Neel}}x \sinh\{K_0(A_{\text{gap}}x)\}. \tag{3.13}$$

Here we use $A_{\text{gap}} = 1.83$ of (3.6) and treat A_{Neel} as a fitting parameter, because A_{Neel} severely depends on the short wavelength cut-off. Figure 7 shows the finite-size scaling plot of $M\mathcal{O}_{\text{Neel}}(\delta, M)$ versus $M\delta^{2/3}$. We have tried the plot of $M^s\mathcal{O}_{\text{Neel}}(\delta, M)$ versus $M\delta^{2/3}$ around $s = 1$ and found that $s = 1$ exhibits the best universal plot. The full curve shows (3.6) with $A_{\text{Neel}} = 1.72$ which is chosen so that the horizontal part of the curve agree with the scaling plot. The analytical prediction for the Néel correlation agrees with the numerical result very well.

For the finite-size string correlation, we also use the value for $j - l = N/2 = M$. From (2.22) the string correlation scales as

$$M^{1/4}\mathcal{O}_{\text{UD}}(\delta, M) = f_{\text{UD}}(M\delta^{2/3}) \tag{3.14}$$

with

$$f_{\text{UD}}(x) = A_{\text{UD}}x^{1/4} \exp\{K_0(A_{\text{gap}}x)/4\}. \tag{3.15}$$

Figure 8 shows the finite-size scaling plot of $N^{1/4}\mathcal{O}_{\text{UD}}(\delta, M)$ versus $M\delta^{2/3}$. We have also plotted $M^{\mu}\mathcal{O}_{\text{UD}}(\delta, M)$ versus $M\delta^{2/3}$ around $\mu = \frac{1}{4}$ for a check and found that the best universal fit is given by $\mu = \frac{1}{4}$. Equation (3.15) is shown by the full curve, where $A_{\text{UD}} = 0.90$ so that the height of the horizontal part of the full curve and the data plot coincide. In figure 8, the difference between the analytical and numerical results is serious for $M\delta^{2/3} > 0.1$.

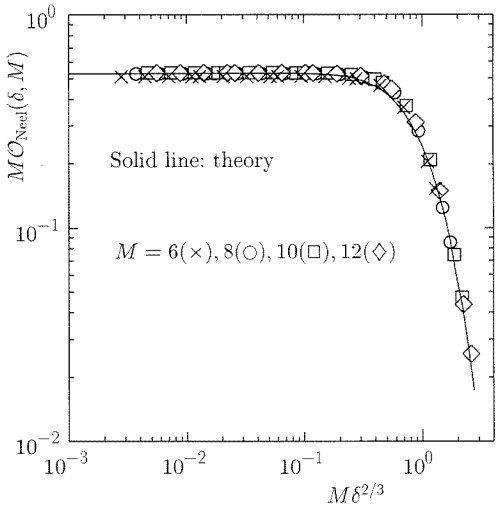

Figure 7. Finite-size scaling plot of $\mathcal{O}_{\rm Neel}(\delta, M)$.

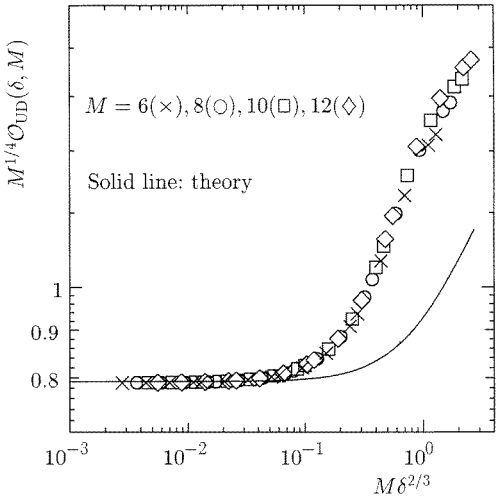

Figure 8. Finite-size scaling plot of $\mathcal{O}_{\rm UD}(\delta, M)$.

4. Discussion

We have investigated the critical behaviours of $\mathcal{H}_0 + \mathcal{H}_1$ for $J_2 = J_{2c} = 0.2411$ and $\delta \to 0$, both analytically and numerically. For the energy gap and the Néel correlation, the analytical expressions explain the numerical results very well (not only their critical exponents but also their amplitudes), although the cut-off-dependent numerical constants in the analytical expressions are treated as fitting parameters. Unfortunately, on the other hand, the analytical approach is less successful for the energy gain and the string correlation.

The analysis of the numerical data brings about

$$G(\delta) \sim \delta^{4/3} |\log \delta| \tag{4.1}$$

because it provides better finite-size scaling than the pure power-law. Further, this exponent $\frac{4}{3}$ is consistent with the hyperscaling relation $a = 2\nu$. Although Chitra *et al* [18] concluded $\nu = 0.667 \pm 0.001$ and $a = 1.251 \pm 0.001$ from their numerical data of DMRG, their exponents do not satisfy the hyperscaling relation $a = 2\nu$.

Let us consider the origin of the logarithmic correction in (4.1). In the uniform XY model without the next-nearest-neighbour interactions, the dispersion relation of the spinless fermion is

$$\Omega(k) = \cos k \tag{4.2}$$

which results in the ground-state energy

$$E_0 = N\int_{-\pi/2}^{\pi/2} \cos k \frac{\mathrm{d}k}{2\pi} = -\frac{N}{\pi}. \tag{4.3}$$

For the uniform Heisenberg model with only nearest-neighbour interactions, the ground-state energy obtained from the Bethe ansatz is

$$E_0 = -\frac{N}{4} - N\int_{-\pi}^{\pi} (1-\cos k)A(k)\mathrm{d}k = -N\left(\frac{1}{4} - \log 2\right) \tag{4.4}$$

where $A(k)$ is the density of states of the wavenumber k. The essential part of (4.3) is similar to (4.2). Although the exact solution for the uniform Heisenberg model with next-nearest-neighbour interactions is unknown, the ground-state energy may have a form like (4.3). When the bond alternation is introduced, the gap δ appears and the dispersion relation of the XY model (4.1) changes into

$$\Omega(k) = \sqrt{\cos^2 k + \delta^2 \sin^2 k}. \tag{4.5}$$

Since the important contribution of the δ-dependence of the energy gain comes from near $k = \pi/2$, we see

$$G(\delta) \sim \int_0^Q \sqrt{q^2+\delta^2}\frac{\mathrm{d}q}{2\pi} \sim \delta^2|\log\delta| \tag{4.6}$$

where $q = \pi - k$ and Q is the upper cut-off. Of course, the integral of $\Omega(k)$ in (4.4) can be expressed by the elliptic integral of the second kind, which also leads to (4.5). In the Heisenberg case, the gap is $v_s q_c \sim \delta^\nu$. Then, if the 'dispersion relation' $\cos k$ in (4.3) is replaced by $\sqrt{q^2+q_c^2}$ near $q = \pi/2$, we can obtain

$$G(\delta) \sim q_c^2|\log q_c| \sim \delta^{2\nu}|\log\delta|. \tag{4.7}$$

The excitation spectrum of the bosonized Hamiltonian also suggests the logarithmic correction in $G(\delta)$. Since the variable θ and P in (2.5) describes the boson field, the ground-state energy is the sum of the zero-point contribution of each mode

$$\frac{1}{2}\int_{-Q}^{Q} v_s\sqrt{q^2+q_c^2}\frac{\mathrm{d}q}{2\pi} \tag{4.8}$$

which also brings about $q_c^2|\log q_c| \sim \delta^{2\nu}|\log\delta|$. However, such a $\delta^{2\nu}|\log\delta|$ contribution is just cancelled out in the course of the SCHA calculation. This complete cancellation seems to be characteristic of the SCHA.

For the string correlation, the analytical expression correctly predicts its critical exponent, but not its amplitude. As can be seen from (2.21), the string correlation includes the S^z operators for the spins between j and l. In the bosonization theory, the S_j^z operator is expressed as the sum of two components, the first is proportional to $\nabla\theta$ (so-called $k \sim 0$ part) and the second to $\sin\theta$ ($k \sim 2k_F$ part) [22]. In the course of the calculation of $\mathcal{O}_{UD}(j-l)$ [21, 23], only the $\nabla\theta$ part are taken into account. Then we guess that this fact brings about the difference between analytical and numerical results. We note that the $k \sim 2k_F$ part is important for the Néel correlation [22].

Recently Brehmer *et al* [29] reported $\nu = 0.862$ for $J_2 = 0.15$ and $\nu = 0.795$ for $J_2 = 0.22$ by using the extrapolated energy gap data obtained from the numerical diagonalization. Their analysis was based on the assumption of the simple algebraic dependence of the gap on δ. They stated that their values of ν was J_2-dependent and is somewhat larger than the predicted value $\nu = \frac{2}{3}$. This difference comes from the existence of the logarithmic correction stated in section 1. The influence of the logarithmic correction becomes smaller as $J_2 \to J_{2c}$, where the logarithmic correction vanishes. Thus, their ν for $J_2 = 0.795$ becomes nearer to $\frac{2}{3}$ than that for $J_2 = 0.15$.

Acknowledgments

We would like to thank H Nishimori for his numerical diagonalization package TITPACK version 2. Part of the numerical calculations were done by using the supercomputer at the Institute of Solid State Physics, University of Tokyo. This work was partly supported by the Grant-in-Aid for Scientific Research (c)(2) no 08640479, from the Ministry of Education, Science, Sports and Culture, Japan.

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