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A Numerical Study of Spin-1/2 Alternating Antiferromagnetic Heisenberg Linear Chains

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We numerically caculate the exact ground state energy $E_0(N, \delta)$ and the first excited state energy $E_1(N, \delta)$ of the one-dimensional spin-$\frac{1}{2}$ alternating antiferromagnetic Heisenberg model

$$H=J\sum_i [1+(-1)^i\delta]S_iS_{i+1}, \quad J>0, \quad 0\leq\delta<1,$$

for $N=8, 10, \cdots, 20$ with N being the number of spins. We employ the finite-size scaling method to determine the critical exponents a, b and ν of the energy gain by alternation, the energy gap and the correlation length as defined by

$$\lim_{N\to\infty} [E_0(N, 0)-E_0(N, \delta)]/N\sim\delta^a, \quad \lim_{N\to\infty} [E_1(N, \delta)-E_0(N, \delta)]\sim\delta^b,$$

and $\xi\sim\delta^{-\nu}$ (ξ is the correlation length), respectively. The estimated values are $a=1.37\pm0.09$, $b=0.79\pm0.06$, $\nu=0.75\pm0.06$. We also analytically calculate ξ and ν by the use of the phase Hamiltonian method for comparison with our numerical result.

§1. Introduction

The one-dimensional (1-d) spin-1/2 alternating antiferromagnetic (AF) Heisenberg system has been attracting increasing attention, especially in relation to the spin-Peierls transition.[1] The Hamiltonian of this system is

$$H=J\sum_i [1+(-1)^i\delta]S_iS_{i+1}, \quad J>0, \tag{1.1}$$

where δ ($0\leq\delta<1$) represents the degree of bond alternation. When $\delta>0$, it is expected that the spins S_{2i} and S_{2i+1} effectively form a singlet pair at low temperatures because the interaction within the pair $J(1+\delta)$ is larger than that between neighbouring pairs $J(1-\delta)$. The decrement of the ground state energy due to this formation of singlet pairs will be expressed as $A\delta^a$ with A, $a>0$ as far as $\delta\ll1$. This quantity is often called the energy gain by alternation. In the spin-Peierls system, of which the above Hamiltonian (1.1) represents the spin degree of freedom, the bond alternation is caused by the periodic lattice distortion paying the energy proportional to δ^2. In the classical treatment of the lattice, the energy change ΔE (per spin) of the spin-Peierls system due to the dimerization is expressed as

$$\Delta E=-A\delta^a+B\delta^2, \quad \text{when} \quad \delta\ll1, \tag{1.2}$$

where B is a positive constant. Therefore the exponent a is of special interest: If $a<2$, the uniform state is unstable and the ground state is spontaneously dimerized. The relation $a<2$ seems to be established because all the existing theories predict $a<2$.

The 1-d spin-1/2 Heisenberg system can be transformed into the interacting spinless Fermion system through the Jordan-Wigner transformation. Many authors[2-12] employed the Hartree-Fock approximation to the resulting interacting spinless Fermion system. In contrast Cross and Fisher[13] used the Boson representation of the Fermion operators. Nakano and Fukuyama[14,15] and Inagaki and Fukuyama[16] refined the method of Cross and Fisher employing the phase representation of the Fermion operators. The renormalization group techniques were also used.[17-22] Duffy and Barr[23] (DB), Matuyama and Okwamoto[20] (MO), Bonner and Blöte[24] (BB), Ramasesha and Soos[25,26] (RS) and Soos, Kuwajima and

Mihalick[27] (SKM) numerically calculated the exact energies of finite systems and extrapolated them to the thermodynamical limit. The quantum Monte-Carlo method was applied by Nakamura, Sogo and Uchinami[28] in the spinless Fermion representation but their results are not precise enough to determine the exponent a.

The existing theoretical predictions are summarized in Table I. Here b is the exponent of the excitation gap of the alternating system. The precise values of a and b are still controversial. Cross and Fisher[13] claims the exactness of their values, but their argument does not go beyond a plausible conjecture. Disagreement between various numerical results is also noticeable. This disagreement seems to come from the difference in the range of δ in the extrapolated energy gain from which the exponent a is determined. In consideration of these situations we thought it worthwhile to perform a numerical analysis similar to those of DB, MO, BB, RS and SKM and to establish a systematic method of extracting the properties of infinite systems from the calculated data of finite systems.

Using a computer program recently developed by Oguchi, Nishimori and Taguchi,[29] we exactly calculated the energy gains due to the alternation and the excitation gaps for systems with $N \leq 20$. By the use of the finite-size scaling method[30] we estimated not only a and b but also the exponent of the correlation length (ν), the last of which was not obtained by the previous numerical calculations. We reexamined the simple extrapolation method used in the previous studies in the light of the finite-size scaling theory. A straightforward application of the resulting extrapolation formula yielded a value of a close to that estimated by the direct finite-size scaling analysis. We also analytically calculated the correlation function $\langle S_i^z S_j^z \rangle$ and the exponent ν by the phase Hamiltonian method for comparison with our numerical results.

§2. Finite-Size Scaling Analysis

Since our method of the numerical calculations is described in ref. 29, we do not enter into the details. Let us just mention here that we did not obtain any information on the total spin quantum number since we reduced the size of matrices by using the conservation of only the z-component of the total spin. The total spin quantum number (not its z-component) plays an important role in characterizing various energy levels as discussed by BB.[24] This type of argument is beyond our present

Table I. Summary of the existing theoretical predictions.

Method		a	b	Reference(s)
Hartree-Fock approximation		2–0	1–0	2–12)
Boson representation		4/3	2/3	Cross & Fisher[13]
Phase Hamiltonian		4/3	2/3	Nakano & Fukuyama[14,15] Inagaki & Fukuyama[16]
Renormalization group		1.3744		Braak *et al.*[17]
		$1.36^{+0.01}_{-0.02}$	0.76	Fields[18] Fields, Blöte & Bonner[19]
		1.78	0.96	Matsuyama & Okwamoto[20]
		4/3+0		Black and Emery[21]
		(*)		Dassen & Moura[22]
Numerical	$N \leq 12$	4/3		Duffy & Barr[23]
	$N \leq 12$	$1.68^{+0.13}_{-0.36}$		Matsuyama & Okwamoto[20]
	$N \leq 12$	1.36±0.1		Bonner & Blöte[24]
	$N \leq 20$	1.72±0.2	0.9±0.1	Ramasesha & Soos[25,26]
	$N \leq 26$	1.6 or 4/3+0	0.9	Soos, Kuwajima & Mihalik[27]

* $G(\infty, \delta) \sim \delta^{4/3}\,(1-0.008 \ln \delta + 0.001 \ln^2 \delta)$

When the energy gain is expressed as $A\delta^2\,|\log \delta|^s$ (s being a positive constant), for instance, we write the exponent a as $a=2-0$. Duffy and Barr[23] themselves did not mention the exponent a. Cross and Fisher[13] pointed out that the data of DB can be interpreted as $a=4/3$.

scope.

We numerically calculated the energy of the ground state $E_0(N, \delta)$ and that of the first excited state $E_1(N, \delta)$ of the Hamiltonian (1.1) with the periodic boundary condition for $N=8, 10, 12, \cdots, 20$ and $0 \leq \delta \leq 0.1$. The energy gain $G(N, \delta)$ (per spin) due to the bond alternation and the excitation gap $\varepsilon_g(N, \delta)$ are expressed as

$$G(N, \delta)=[E_0(N, 0)-E_0(N, \delta)]/N, \quad (2.1)$$

$$\varepsilon_g(N, \delta)=E_1(N, \delta)-E_0(N, \delta), \quad (2.2)$$

respectively. We analyzed the data of $G(N, \delta)$ and $\varepsilon_g(N, \delta)$ by the finite-size scaling theory.

When $\delta=0$ the equal-time correlation function of S^z is of power decay type,[31] i.e.,

$$\langle S_i^z S_j^z \rangle \sim |x_i-x_j|^{-1}, \quad (2.3)$$

whereas when $\delta \neq 0$ it is expected that

$$\langle S_i^z S_j^z \rangle \sim |x_i-x_j|^{-m} \exp[-|x_i-x_j|/\xi], \quad (2.4)$$

where m is a positive constant, ξ the correlation length and x_i the location of the i-th spin (see Appendix). Since the power decay of eq. (2.3) is a result of the divergence of ξ at $\delta=0$ in eq. (2.4), we can write ξ as

$$\xi \sim \delta^{-\nu}, \quad (\nu>0), \quad (2.5)$$

which defines the exponent ν. Therefore our problem is a critical phenomenon in which the critical point is at $\delta=0$. In the XY system, however, $\delta=0$ is not the critical point because it is easily proved that $\langle S_i^z S_j^z \rangle$ is of power decay type even when $\delta>0$. Hence we consider only the Heisenberg system throughout this paper.

In the finite-size scaling theory,[30] it is assumed that a physical quantity $P(N, \delta)$ obeys the scaling law

$$P(N, \delta) \sim N^{\omega} p(N/\xi)=N^{\omega} p(x), \quad x=N/\xi, \quad (2.6)$$

as far as $N \gg 1$ and $\delta \ll 1$. We apply this relation to $G(N, \delta)$ and $\varepsilon_g(N, \delta)$,

$$G(N, \delta) \sim N^u g(x), \quad (2.7)$$

$$\varepsilon_g(N, \delta) \sim N^w f(x). \quad (2.8)$$

From the required limiting behaviors of $G(N, \delta)$ and $\varepsilon_g(N, \delta)$

$$G(\infty, \delta) \sim \delta^a, \qquad G(N, 0)=0, \quad (2.9)$$

$$\varepsilon_g(\infty, \delta) \sim \delta^b, \qquad \varepsilon_g(N, 0) \sim N^{-c}, \quad (2.10)$$

we obtain

$$G(N, \delta) \sim N^{-a/\nu} g(x), \quad (2.11)$$

$$g(x) \sim \begin{cases} 0 & (x \to 0) \\ x^{a/\nu} & (x \to \infty) \end{cases}, \quad (2.12)$$

and

$$\varepsilon_g(N, \delta) \sim N^{-c} f(x), \quad (2.13)$$

$$f(x) \sim \begin{cases} \text{const.} (>0) & (x \to 0) \\ x^c & (x \to \infty) \end{cases}, \quad (2.14)$$

as well as

$$c=b/\nu. \quad (2.15)$$

Now we determine the critical exponents successively by the following procedure:

(a) We can easily determine the exponent c from a log-log plot of $\varepsilon_g(N, 0)$ as a function of N.

(b) As is seen from eq. (2.13), the quantity $\varepsilon_g(N, \delta)N^c$ is a universal function of $x=N\delta^\nu$. Therefore we can determine ν so that a plot of $\varepsilon_g(N, \delta)N^c$ as a function of x is universal.

(c) By the use of the value of ν determined in (b), the exponent a is determined so that a plot of $G(N, \delta)N^{a/\nu}$ as a function of x is universal as in eq. (2.11).

A log-log plot of $\varepsilon_g(N, 0)$ versus N is shown in Fig. 1, from which we obtain $c=b/\nu=0.95$ within the fitting error less than 0.01. In Fig. 2

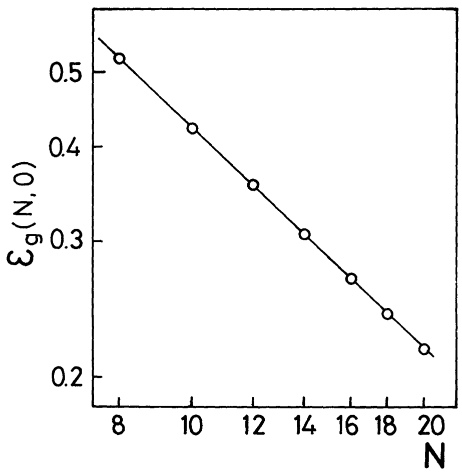

Fig. 1. A log-log plot of $\varepsilon_g(N, 0)$ as a function of N. The energy unit is J.

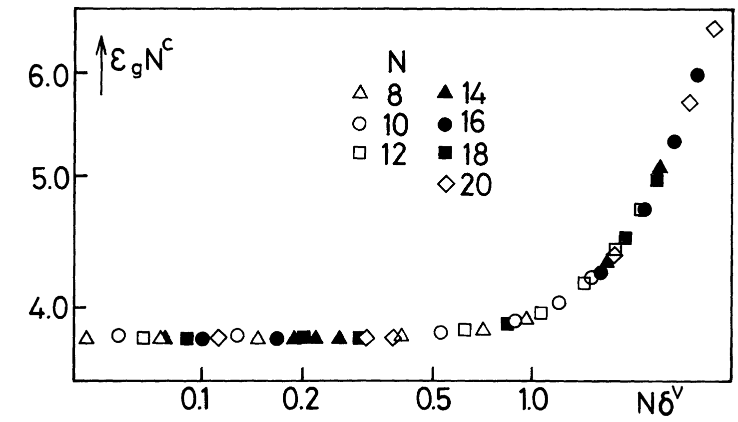

Fig. 2. A log-log plot of $f(x)=\varepsilon_g(N, \delta)N^c$ versus $x\equiv N\delta^\nu$ for $0.01\le\delta\le0.1$.

we show $f(x)=\varepsilon_g(N, \delta)N^c$ as a function of $x=N\delta^\nu$ when $\nu=0.79$, which gives the best fit for all over the region of x. Therefore the function $f(x)$ is universal for wide range of x. The behavior of $f(x)$ is clearly different between in $x<1$ region and in $x>1$ region, which is expected from eq. (2.14). If we choose a wrong value for ν, the universal curve splits into different curves for various N. Since the data points are scattered significantly when $\nu<0.77$ or $\nu>0.81$, the value of ν is estimated as $\nu=0.79\pm0.02$. A plot of $g(x)=G(N, \delta)N^{a/\nu}$ as a function of $x=N\delta^\nu$ is shown in Fig. 3. In this case the difference of the behavior of $g(x)$ in two regions ($x>1$ and $x<1$) is not so clear because $g(x)\sim x^{a/\nu}$ when $x\gg1$ and $g(x)\sim x^{2/\nu}$ when $x\ll1$ (see §3). For this function similar scatterings of data points were observed when a deviated from the best-fit value by 0.02. We estimated a as $a=1.37\pm0.02$.

These error estimations should not be regarded as final ones. It may happen that the scaling relations (2.11)-(2.14) are satisfied before fully entering into the critical region of interest. If this is the case, the present analysis could give incorrect critical exponents with apparently small errors. We return to this point in the next section.

§3. Discussion

In the preceding section we have obtained the exponents a, b and ν by the use of the finite-size scaling theory. To check the reliability of the values of the exponent a and the

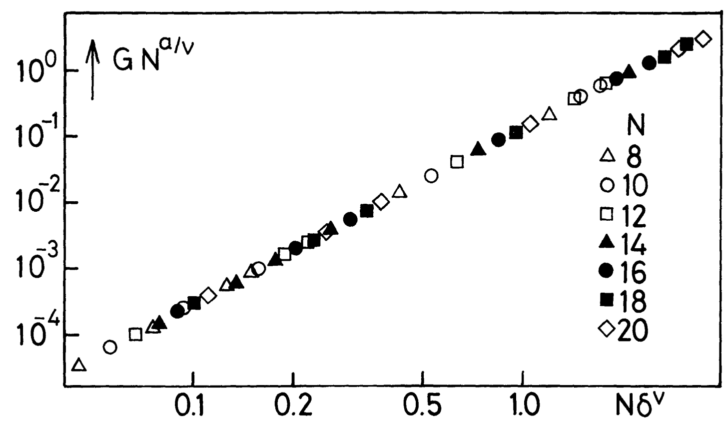

Fig. 3. A log-log plot of $g(x)=G(N, \delta)N^{a/\nu}$ as a function of $x\equiv N\delta^\nu$ for $0.01\le\delta\le0.1$.

finite-size scaling hypothesis, for the exponent a we also applied the simple extrapolation method used by the previous numerical studies. As the extrapolation formula we used

$$G(N, \delta)=G(\infty, \delta)+\sum_{i=1}^{n}\frac{h_i(\delta)}{N^i}, \qquad (3.1)$$

which is one of the formulae giving the best fit when $\delta\ll 1$ according to BB. As shown in Fig. 4, the extrapolated energy gain $G(\infty, \delta)$ obeys the $\delta^{4/3}$-law for $0.04\leq\delta\leq 0.1$. This confirms the results of BB ($a\simeq 4/3$ for $\delta\geq 0.03$), MO ($a\simeq 1.31$ for $\delta\gtrsim 0.1$) and SKM ($a\simeq 4/3$ for $\delta\gtrsim 0.05$). However, if δ approaches the critical point $\delta=0$, the exponent a rapidly converges to 2. This fact is interpreted in the following discussion.

Although BB employed the extrapolation formula (3.1) on empirical grounds, it is possible to derive it from the finite-size scaling hypothesis. The $N\to\infty$ extrapolation with fixed δ corresponds to taking the limit $x\equiv N\delta^{\nu}\to\infty$ in eq. (2.12). Since it is expected that the scaling function $g(x)$ is well-behaved, the asymptotic form of $g(x)$ when $x\to\infty$ will be

$$g(x)\sim x^{a/\nu}(1+g_1x^{-1}+g_2x^{-2}+\cdots). \qquad (3.2)$$

Therefore, when $N\to\infty$ with fixed δ, the function $G(N, \delta)$ behaves as

$$G(N, \delta)\sim G(\infty, \delta)\left[1+\frac{g_1\delta^{-\nu}}{N}+\frac{g_2\delta^{-2\nu}}{N^2}+\cdots\right], \qquad (3.3)$$

which is equivalent to eq. (3.1). Of course the correct value of $G(\infty, \delta)$ is obtained by the use of eq. (3.3) only when $x=N\delta^{\nu}>1$, which explains the incorrect value $a=2$ (not 4/3) at $\delta\leq 0.04$ in Fig. 4. This incorrect value $a=2$ is a natural result from the applicability of the perturbational expansion with respect to δ in a finite system and the symmetry of the present system (with even N and the periodic boundary condition) against the replacement $\delta\to-\delta$. For a system without this symmetry the incorrect value of a will be 1 instead of 2. From the δ^2 dependence of $G(N, \delta)$ in the $x<1$ region it follows that $g(x)\sim x^{2/\nu}$ as $x\to 0$. The present situation is schematically shown in Fig. 5. To obtain the correct value of $G(\infty, \delta)$ the extrapolation $N\to\infty$ must be done in the $x>1$ region. SKM found that $a\simeq 4/3$ for $\delta\geq 0.05$ and $a\simeq 1.6$ for $\delta\leq 0.05$ and claimed that $a\simeq 1.6$ is the correct exponent. They actually recognized that the data for $\delta\leq 0.05$ seriously reflect the finite size effects. In order to remedy this drawback, they invented an elaborate extrapolation formula using both even and odd N data. However, we stress that, for the purpose of predicting exponents, any extrapolation is invalid in the region $\delta\lesssim 0.05$ if $N\leq 26$. We believe that their value $a\simeq 1.6$ is dragged by the above-mentioned incorrect values $a=2$ for even N and $a=1$ for odd N. We note that in our finite-size scaling method the wider range of data (from $x\ll 1$ to $x\gg 1$) were used to determine the exponents, whereas only those of $x\gg 1$ should be taken

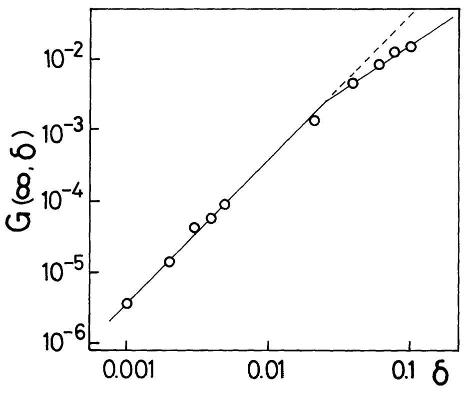

Fig. 4. Extrapolated energy gain $G(\infty, \delta)$ by the use of eq. (3.1) with $n=3$. The quantity $G(\infty, \delta)$ behaves as $G(\infty, \delta)\sim\delta^{4/3}$ when $\delta\geq 0.04$ while $G(\infty, \delta)\sim\delta^2$ when $\delta\leq 0.02$.

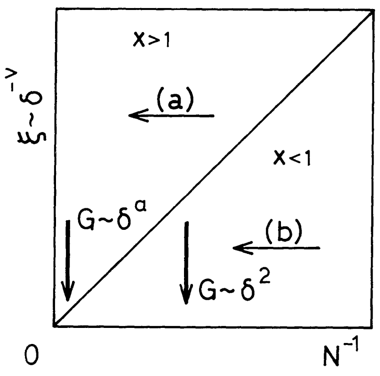

Fig. 5. A sketch of the $x>1$ and $x<1$ regions. The extrapolation $N\to\infty$ with fixed δ leads to correct value of a in (a) case while to incorrect value in (b) case. These cases correspond to $\delta\geq 0.04$ and $\delta\leq 0.02$ in Fig. 4, respectively.

into account in the extrapolation method. Another advantage of the finite-size scaling method is its capability to predict the values of b and ν. The simple extrapolation method[20,23,24] fails to estimate b because of poor convergence of the energy gap. The exponent ν is out of scope of the extrapolation method from the outset as far as only the data of $G(N, \delta)$ and $\varepsilon_g(N, \delta)$ are used.

It is worthwhile to point out a remarkable feature of

$$c = b/\nu. \tag{3.4}$$

This equation connects the exponents (b and ν) of the alternating infinite system with that (c) of the uniform finite system. Since the relation (3.4) is derived from eqs. (2.5) and (2.10) and the finite-size scaling hypothesis without reference to the specific form of the Hamiltonian (1.1), this relation is expected to hold good not only for the present system but also for any 1-d spin-1/2 AF Heisenberg system with a perturbation which brings about an excitation gap and a finite correlation length. Equation (3.4) may be interpreted as an example of weak universality:[32] The exponent b scaled by ν assumes a universal value for any perturbation of the type described above.

Although $c=0.95$ in our numerical calculation, the exact value will be $c=1$ because the low lying excitation spectrum of the uniform ($\delta=0$) and infinite AF system is[33] $\omega(q) = 2\pi J|\sin q|$ and the smallest non-zero q is of order $1/N$ for a finite system, which implies $\varepsilon_g(N, 0) \sim O(1/N)$ as $N \to \infty$. If this is the case, it follows from eq. (3.4) that $b=\nu$. A physical interpretation of $b=\nu$ is possible. Since the low lying excitation will be the spin wave excitation (see Appendix), the energy gap ε_g will be expressed as $\varepsilon_g \sim v_s/l$, where v_s is the spin wave velocity and l is a quantity of the dimension of length. If there is only one characteristic length in this system, which we implicitly assumed in the finite size scaling equation, we can interpret l as the correlation length ξ. Thus the exponents of ε_g and ξ coincide if v_s is not seriously renormalized due to the alternation. The above mentioned situation can be seen in Appendix where ξ is calculated by the use of the phase Hamiltonian.

As has been already stated our numerical calculation leads to $c=0.95$ whereas the exact value is expected to be $c=1$. This fact suggests that even our $N=20$ system is not sufficiently large as far as the uniform case ($\delta=0$) is concerned. In §2 we estimated the errors of the exponents as ± 0.02, where we have not considered the possible fact that our systems are not large enough to determine the accurate exponents. In other words, there is a possibility that our systems are not deeply in the critical region where the finite-size scaling analysis yields the correct exponents. Unfortunately we have no systematic way to estimate the errors of the exponents due to this effect. We performed the same analysis as in §2 with data only for $N \leq 16$ to see if there is apparent dependence of the exponents on the system size. But we could not observe it. Here we conveniently estimate the errors of exponents as 5%, which reflects the deviation of $c=0.95$ from the exact value $c=1$. For instance, we estimate a as $(1.37-0.02)\times 0.95 \leq a \leq (1.37+0.02)\times 1.05$, since we estimated $a=1.37\pm 0.02$ in §2. Then we can write

$$\left.\begin{aligned} a &= 1.37 \pm 0.09, \\ b &= 0.79 \pm 0.06, \\ \nu &= 0.75 \pm 0.06. \end{aligned}\right\} \tag{3.5}$$

We also carried out numerical analysis with free boundary to check further the effects of finiteness of our system. The results are

$$\left.\begin{aligned} &a = 1.41 \pm 0.21, \quad b = 0.71 \pm 0.11, \\ &\nu = 0.85 \pm 0.13, \quad c = 0.85 \quad (+0.15). \end{aligned}\right\} \tag{3.6}$$

The errors of 15% have been added because of the deviation of $c=0.85$ from $c=1$.

Our final estimation of the exponents is in eq. (3.5). For the exponent a, the predictions by the Boson method (or the phase Hamiltonian approach) and by the renormalization group (RG) treatment show good agreement with each other and with our result. On the other hand, for the exponent b, the predictions by the existing two methods are slightly different from each other: $b=2/3$ by Boson method (or the phase Hamiltonian approach) and $b=0.76$ by the RG treatment. Our numerical calculation seems to support the latter rather than the former. Further investigations are required to determine the values of b and ν.

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Appendix: Calculation of $\langle S_i^z S_j^z \rangle$ by the Phase Hamiltonian Method

We begin with the phase Hamiltonian of Nakano and Fukuyama[14,15] (NF),

$$H=\int \mathrm{d}x[A(\nabla\theta)^2+CP^2-B\cos\theta+D\cos 2\theta], \tag{A·1}$$

where*

$$A=Jd/4, \quad C=\pi^2 Jd,$$
$$B=2J\pi/d, \quad D=\pi^2 J/4d, \tag{A·2}$$
$$[\theta(x), P(x')]=i\delta(x-x'), \tag{A·3}$$

and d is the spin spacing. In the self-consistent harmonic approximation (SCHA), the approximated Hamiltonian is

$$H_{\mathrm{SCHA}}=\int \mathrm{d}x[A(\nabla\theta)^2+CP^2+Aq_0^2\theta^2], \tag{A·4}$$

with

$$Aq_0^2=\frac{1}{2}B\exp\left(-\frac{1}{2}\langle\theta^2\rangle\right)-2D \times\exp(-2\langle\theta^2\rangle), \tag{A·5}$$

and the excitation of this Hamiltonian is given by

$$\omega(q)=v_{\mathrm{s}}\sqrt{q^2+q_0^2}. \tag{A·6}$$

Therefore the excitation gap is $v_{\mathrm{s}}q_0$, which is nothing but ε_{g}.

The spin density $S^z(x)$ in the continuum approximation is written as[16,27]

$$S^z(x)=\frac{1}{d}\sin\left(\frac{\pi}{d}x+\theta\right)+\frac{1}{2\pi}\nabla\theta, \tag{A·7}$$

where the first (second) term represents the fast (slow) varying part and S_i^z should be expressed as

$$S_i^z=\int_{x_i-d/2}^{x_i+d/2} \mathrm{d}x S^z(x), \tag{A·8}$$

with x_i being the position of the i-th spin. The correlation function of $S^z(x)$ is

$$D(x,x')\equiv\langle S^z(x)S^z(x')\rangle =D_1(x,x')+D_2(x,x'), \tag{A·9}$$

$$D_1(x,x')\equiv d^{-2}\langle\sin[(\pi x/d)+\theta(x)] \times\sin[(\pi x'/d)+\theta(x')]\rangle, \tag{A·10}$$

$$D_2(x,x')\equiv(1/4\pi^2)\langle\nabla\theta(x)\nabla\theta(x')\rangle. \tag{A·11}$$

It is convenient to introduce the Green's function

$$G(x,x',t)=G(x-x',t) \equiv\langle T_t\theta(x,t)\theta(x',0)\rangle. \tag{A·12}$$

Since its Fourier transform $G(q,\omega)$ is easily calculated as

$$G(q,\omega)=2C/[\omega^2+v_{\mathrm{s}}^2(q^2+q_0^2)], \tag{A·13}$$

we obtain

$$G(x,x',t)=(C/\pi v_{\mathrm{s}})K_0(\sqrt{q_0^2(x-x')^2+v_{\mathrm{s}}^2t^2}), \tag{A·14}$$

where $K_n(z)$ is the n-th order modified Bessel function.

From eqs. (A·11), (A·12) and (A·14) we get

$$D_2(x,x')=(q_0^2/8\pi^2)[K_0(q_0|x-x'|)+K_2(q_0|x-x'|)] \sim(\sqrt{\pi}q_0^2/4\sqrt{2})(q_0|x-x'|)^{-\frac{1}{2}}\exp(-q_0|x-x'|),$$

when

$$q_0|x-x'|\gg 1. \tag{A·15}$$

Due to the harmonic nature of H_{SCHA}, it follows that

* As can be seen from eq. (1.1), the interaction $2J$ in our paper corresponds to J in the paper of NF.

$$\langle T_t \exp[i\theta(x,t)] \exp[\pm i\theta(x',0)]\rangle = \exp[-G(x-x',t) \mp G(0,0)]$$
$$= (dq_0/2\pi) \exp[\mp K_0(\sqrt{q_0^2(x-x')^2+v_s^2 t^2})], \quad (\mathrm{A}\cdot 16)$$

where for $G(0, 0)$ we have performed the q-integral in the region $|q|<\pi/d$ to remove the unphysical divergence. Then $D_1(x, x')$ becomes

$$D_1(x,x') = (q_0/4\pi d)\{\cos[\pi(x-x')/d] \exp[K_0(q_0|x-x'|)]$$
$$-\cos[\pi(x+x')/d] \exp[-K_0(q_0|x-x'|)]. \quad (\mathrm{A}\cdot 17)$$

Integrating eqs. (A·15) and (A·17), we finally obtain

$$\langle S_i^z S_j^z\rangle = [(-1)^{i-j}\sqrt{2}\pi^{-2/5} dq_0 + 2^{-1/2}\pi^{-3/2}(dq_0)^2](q_0|x_i-x_j|)^{-1/2} \exp(-q_0|x_i-x_j|)$$
$$\sim (-1)^{i-j}\sqrt{2}\pi^{-5/2} dq_0 (q_0|x_i-x_j|)^{-1/2} \exp(-q_0|x_i-x_j|), \quad (\mathrm{A}\cdot 18)$$

where we have used the fact $dq_0 \ll 1$. The correlation length ξ is expressed as

$$\xi = 1/q_0 = v_s/\varepsilon_g. \quad (\mathrm{A}\cdot 19)$$

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