Spin correlation function of the $S=1$ antiferromagnetic Heisenberg chain by the large-cluster-decomposition Monte Carlo method

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We calculate correlation functions of a one-dimensional spin $S=1$ antiferromagnetic Heisenberg model by the large-cluster-decomposition Monte Carlo method. We find that the correlation functions are well approximated by modified Bessel functions. This result supports Haldane's conjecture, and the correlation length agrees with that obtained from spin-wave theory using elementary excitation data.

I. INTRODUCTION

Since Haldane conjectured in 1983 (Ref. 1) that the integer antiferromagnetic spin chain, in contrast with the half-integer case, has an energy gap and its correlation function decays exponentially, many numerical works have been done. Botet *et al.*[2] carried out exact diagonalization of finite-size systems ($N=2-12$). Their analysis by the finite-size-scaling technique supports Haldane's prediction. But this result is criticized by Bonner and Müller,[3] and independently by Sólyom and Ziman.[4] Bonner and Müller applied the finite-size-scaling technique to the $S=\frac{1}{2}$ case, and they concluded that the finite-size result up to $N=30$ might be required to find the true asymptotic behavior. Recently, Nightingale and Blöte[5] calculated the energy gap up to $N=32$ using a Green's-function Monte Carlo method. They concluded that the energy gap is $0.41J$ in the limit of $N\rightarrow\infty$.

As for the correlation functions, exact calculation was done up to $N=16$ by Moreo,[6] and independently by Natsume and Matsushita.[7] Kubo and Takada[8] applied a quantum-transfer-matrix method for finite temperature to this problem. Extrapolating their results to the ground state, they obtained a finite correlation length and their results are consistent with Haldane's conjecture. Using a checkerboard-decomposition Monte Carlo method, Sogo and Uchinami[9] calculated spin-correlation functions for $N=40$. They analyzed staggered magnetization of $S=1$ XXZ models, and obtained negative results for Haldane's conjecture. A similar calculation was done by Takahashi,[10] but he analyzed the correlation function directly, and his result supports Haldane's conjecture. Recently, Uchinami[11] extended their calculation of staggered magnetization up to $N=80$, and this time his results support Haldane's conjecture.

In this paper, we calculate spin-correlation functions of the $S=1$ antiferromagnetic spin chain by a variant of the checkerboard-decomposition Monte Carlo method.[12]

II. METHOD

We write the antiferromagnetic Heisenberg Hamiltonian as follows:

$$H=\sum_{i=0}^{N-1} h_i,\quad h_i=S_i^xS_{i+1}^x+S_i^yS_{i+1}^y+S_i^zS_{i+1}^z\ ,\qquad \mathbf{S}_N=\mathbf{S}_0\ . \tag{2.1}$$

Using the large-cluster decomposition,[13] we get the following equation for the partition function Z:

$$\begin{aligned} Z&\simeq \mathrm{Tr}[(V_1V_2)^L]\ ,\\ V_1&=\prod_{k=\mathrm{odd}}\exp(-\tau H_k)\ ,\\ V_2&=\prod_{k=\mathrm{even}}\exp(-\tau H_k)\ ,\\ H_k&=\sum_{j=0}^{p-1} h_{pk+j}\ ,\\ \tau&=\beta/L\ , \end{aligned} \tag{2.2}$$

where p is cluster size (see Fig. 1). A Monte Carlo state is represented by a set of $N\times 2L$ classical spins $S_{i,j}^z$ ($i=0,1,\ldots,N-1$, $j=0,1,\ldots,2L-1$). The Boltzmann weight is given by

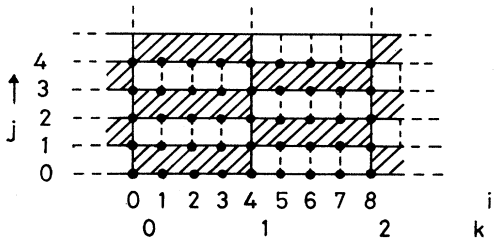

FIG. 1. Graphical representation of the p-spin cluster decomposition in the case $p=4$. Equivalent classical lattice is represented by a checkerboardlike lattice; i denote sites on the original $1-d$ lattice, k is a label of spin cluster p, and j is a label along the Trotter direction. The shaded rectangles denote where $2(p+1)$ local spins interact. The two spins on the sites connected by dashed lines are equal.

$$W(\{S^z_{i,j}\}) = \prod_{k+j=\text{even}} \langle \alpha_{k,j} | \exp(-\tau H_k) | \alpha_{k,j+1} \rangle \ , \qquad |\alpha_{k,j}\rangle \equiv |S^z_{pk,j}, S^z_{pk+1,j}, \ldots, S^z_{p(k+1),j}\rangle \ . \tag{2.3}$$

In a Monte Carlo trial, we employ the two types of updating processes, the inner-block process and corner process. These processes must satisfy local-spin conservation,

$$\sum_{i=0}^{p} S^z_{pk+i,j} = \sum_{i=0}^{p} S^z_{pk+i,j+1} \quad (k+j=\text{even}) \ , \tag{2.4}$$

and the following identity:

$$S^z_{pk+i,j+1} = S^z_{pk+i,j+2} \qquad (k+j=\text{even}, i=1,2,\ldots,p-1) \ . \tag{2.5}$$

These processes are illustrated in Fig. 2. In an inner-block process, we choose new states $\{S'^z_{i,j}\}$ which satisfy

$$\begin{aligned} &\sum_{i=1}^{p-1} S'^z_{pk+i,j} = \sum_{i=1}^{p-1} S^z_{pk+i,j} \ , \\ &S'^z_{pk+i,j+1} = S'^z_{pk+i,j} \quad (i=1,\ldots,p-1) \ , \\ &|S'^z_{i,j}| \le S \ , \\ &S'^z_{pk,j} = S^z_{pk,j}, \quad S'^z_{p(k+1),j} = S^z_{p(k+1),j} \quad (k+j=\text{odd}) \ , \end{aligned} \tag{2.6}$$

and we accept one of the states using the heat-bath method. Similarly, in a left-corner process, we choose new states $\{S'^z_{i,j}\}$ which satisfy

$$\begin{aligned} &S'^z_{pk,j} = S^z_{pk,j} + m \ , \\ &S'^z_{pk,j+1} = S^z_{pk,j+1} + m \ , \\ &S'^z_{pk+1,j} = S'^z_{pk+1,j+1} = S^z_{pk+1,j} - m \ , \\ &|S'^z_{i,j}| \le S \end{aligned} \tag{2.7}$$

(where $k+j$=odd, m=integer), and we accept one of the states using the heat-bath method. Right-corner process can be done in the same way.

In the case of the pair-decomposition Monte Carlo method, it is difficult to take τ small enough to include sufficient quantum effects.[14] Using large-cluster decomposition, one can take account of quantum effects for fairly large τ.

The correlation function of the quantum system is given by

$$\rho(l) \equiv N^{-1} \sum_i \langle S^z_i S^z_{i+l} \rangle = (2NL)^{-1} \sum_{i,j} \langle S^z_{i,j} S^z_{i+l,j} \rangle \ . \tag{2.8}$$

In order to calculate the correlation function, following Takahashi,[10] we use the structure factor $S(q)$:

$$\begin{aligned} &S(q) \equiv \sum_l e^{iql} \rho(l) = (2L)^{-1} \sum_{j=0}^{2L-1} \langle |S^z_{q,j}|^2 \rangle \ , \\ &S^z_{q,j} = N^{-1/2} \sum_m e^{iqm} S^z_{m,j} \ . \end{aligned} \tag{2.9}$$

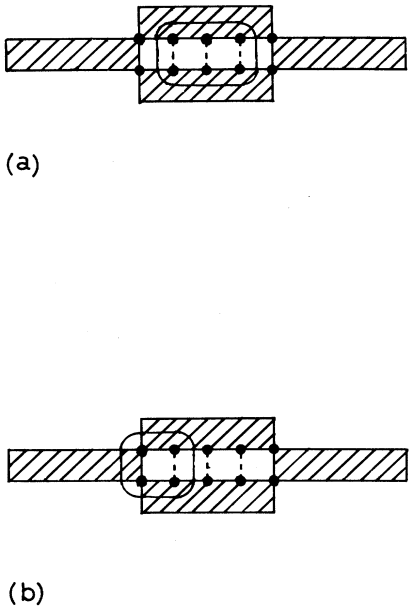

FIG. 2. (a) Inner-block process; (b) corner process. The encircled spins are flipped.

In the sequence of the Monte Carlo simulation we calculate $S(q)$ by the fast Fourier transformation. After Monte Carlo calculation of $S(q)$, we calculate $\rho(l)$ by the inverse Fourier transformation. Using this method, the speed of calculation is faster than the conventional method ($N \log_2 N$ versus N^2).

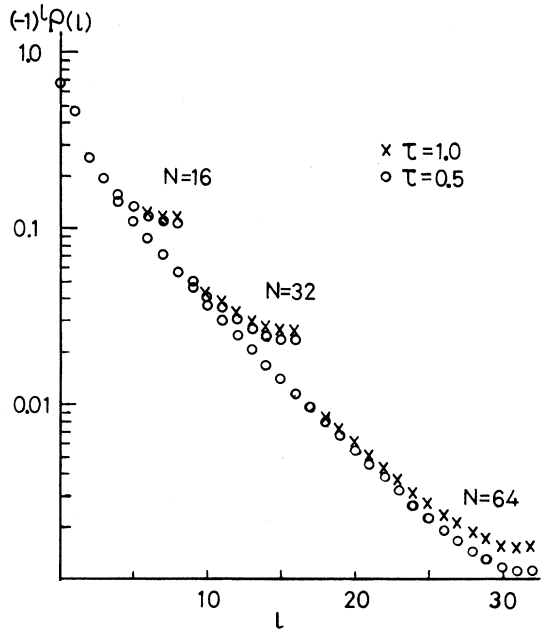

FIG. 3. Spin-correlation function $(-1)^l \langle S^z_i S^z_{i+l} \rangle$ is plotted as a function l in semilog plot. Crosses are for $\tau=1.0$ and circles are for $\tau=0.5$. N means system size. Apparently, the $N=64$ data are nearly on a straight line.

TABLE I. Correlation functions $(-1)^l\rho(l)$ and energy for $N=16$.

l	$\tau=1.0$	$\tau=0.5$	Exact
0	0.6694(6)	0.6692(9)	0.6667
1	0.4786(10)	0.4739(15)	0.4673
2	0.2709(11)	0.2628(16)	0.2538
3	0.2155(10)	0.2083(15)	0.1997
4	0.1670(10)	0.1596(16)	0.1511
5	0.1442(9)	0.1365(14)	0.1273
6	0.1264(8)	0.1184(14)	0.1093
7	0.1186(7)	0.1105(13)	0.1013
8	0.1152(7)	0.1068(14)	0.0973
E_0	22.750(2)	22.543(3)	22.4468

III. RESULTS

We have dealt with the cases $N=16-64$, $\tau=0.5-1.0$, and $\beta=32-64$, which can be regarded practically as zero temperature. We set the cluster size $p=4$. The ratio of inner-block and corner processes is chosen as 4:1. After 2×10^5 Monte Carlo steps for thermalization, we did eight runs with 10^5 Monte Carlo steps. We investigate only the $\sum_{i=0}^{N-1} S^z_{i,j}=0$ subspace, because we are mainly interested in the ground state. In Tables I and II we show the energy and correlation functions for $N=16$ and 64 obtained with the Monte Carlo method. Comparing this result with the exact result,[6,7] the agreement is good. The correlation functions $\rho(l)$ are plotted as a function l in Fig. 3. From Fig. 3 we see that spin-correlation decays almost exponentially, but a semilog plot of $(-1)^l\rho(l)$ shows a slightly upward curvature. As is well known, the $1-d$ quantum system can be mapped onto a $2-d$ classical system.[15] If the original system has an energy gap, its correlation function becomes of the $2-d$ Orstein-Zernike form, that is, the modified Bessel function $K_0(|l|/\xi)$

$$\int \frac{\exp(i\mathbf{q}\cdot\mathbf{l})d^2q}{q^2+\xi^{-2}}=2\pi K_0(|l|/\xi)\ . \tag{3.1}$$

The large-separation correlation becomes, as Haldane suggested, $(-1)^l|l|^{-1/2}\exp(-|l|/\xi)$. Figure 4 shows $|l^{1/2}\rho(l)|$ as a function l in semilog plot. The linearity of the curve is very much improved. In Fig. 5 we compare the fitting of the correlation function in the form $AK_0(|l|/\xi)$ with $A\exp(-|l|/\xi)$ and $A|l|^{-1/2}\exp(-|l|/\xi)$. Apparently the fitting in the form $AK_0(|l|/\xi)$ is best. The estimated inverse correlation lengths $1/\xi$ for the cases $N=64$ and $\tau=1.0,0.5$ are

$$1/\xi=\begin{cases}0.156 & \text{for } \tau=1.0\ ,\\ 0.159 & \text{for } \tau=0.5\ .\end{cases}$$

Using a τ^2 correction law,[16] we extrapolate from these results to the $\tau\to0$ limit,

TABLE II. Correlation functions $(-1)^l\rho(l)$ and energy for $N=64$.

l	$\tau=1.0$	$\tau=0.5$
0	0.6667(1)	0.6671(1)
1	0.4736(1)	0.4701(1)
2	0.2611(2)	0.2549(1)
3	0.2014(2)	0.1963(1)
4	0.1479(2)	0.1427(1)
5	0.1188(2)	0.1135(1)
6	0.0936(2)	0.0883(1)
7	0.0762(2)	0.0713(1)
8	0.0610(2)	0.0567(1)
9	0.0497(2)	0.0461(2)
10	0.0402(2)	0.0373(2)
11	0.0330(2)	0.0306(2)
12	0.0270(2)	0.0249(2)
13	0.0225(2)	0.0206(2)
14	0.0186(2)	0.0170(2)
15	0.0156(2)	0.0142(3)
16	0.0128(2)	0.0116(3)
17	0.0106(2)	0.0096(3)
18	0.0088(3)	0.0080(3)
19	0.0074(3)	0.0067(3)
20	0.0062(3)	0.0055(4)
21	0.0053(3)	0.0047(4)
22	0.0044(3)	0.0039(4)
23	0.0038(4)	0.0033(4)
24	0.0032(3)	0.0027(5)
25	0.0028(3)	0.0023(5)
26	0.0024(3)	0.0019(5)
27	0.0021(3)	0.0017(5)
28	0.0018(4)	0.0015(5)
29	0.0017(4)	0.0013(6)
30	0.0016(4)	0.0012(6)
31	0.0015(4)	0.0011(6)
32	0.0016(4)	0.0011(6)
E_0	90.941(1)	90.119(3)

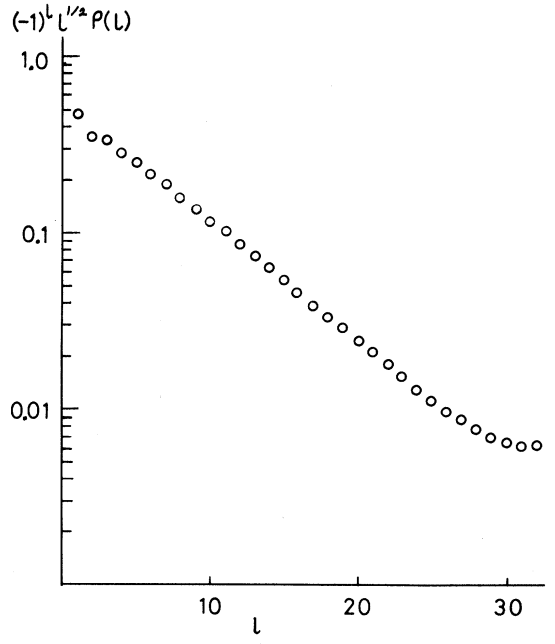

FIG. 4. $(-1)^l l^{1/2}\langle S^z_i S^z_{i+l}\rangle$ is plotted as a function of l in semilog plot. We set here $\tau=0.5$ and $N=64$. Comparing with Fig. 3, the linearity of curve is improved.

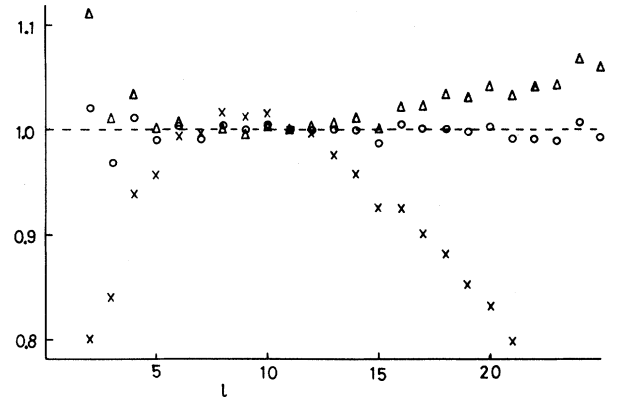

FIG. 5. Comparison of the fittings of the correlation function in the form $AK_0(|l|/\xi)$ with $A\exp(-|l|/\xi)$ and $A|l|^{-1/2}\exp(-|l|/\xi)$. Apparently the fitting in the form $AK_0(|l|/\xi)$ is best. ○, $AK_0(l/\xi)/\rho(l)$; △, $Al^{-1/2}\exp(-l/\xi)/\rho(l)$; ×, $A\exp(-l/\xi)/\rho(l)$.

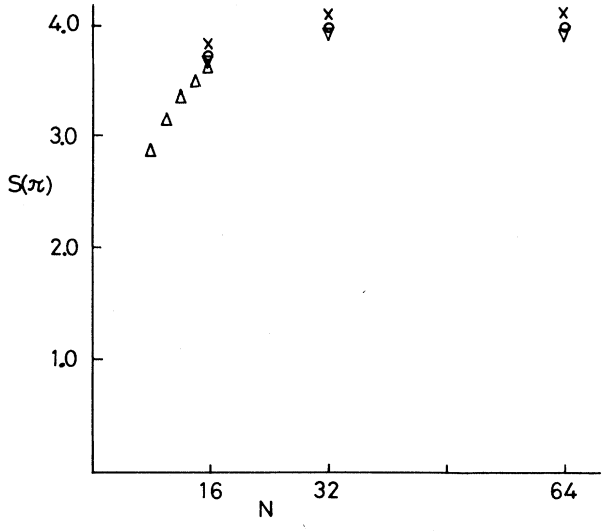

FIG. 7. $S(\pi)$ as a function of system size N. ×, $\tau=1.0$; ○, $\tau=0.5$; ▽, extrapolated data; △, exact results.

$$1/\xi=0.160\ . \tag{3.2}$$

This value is near the results of Takahashi[10] ($1/\xi=0.18$) and Takada[8] ($1/\xi=0.12$).

According to spin-wave theory,[1,10] the elementary excitation of the antiferromagnetic Heisenberg chain is approximated by

$$\varepsilon(q)^2=c^2(\sin^2 q+\xi^{-2})\ , \tag{3.3}$$

where q is the wave number and c is the so-called light velocity of the system. Parkinson and Bonner[17] have calculated the elementary excitation up to $N=14$ by the Lanczös method, and independently Takahashi[18] has calculated the elementary excitation for $N=32$ by the projector Monte Carlo method. From their results in the neighborhood of $q=\pi$ and Eq. (3.3), we estimate that

$$1/\xi=0.165,\quad c=2.57,\quad \varepsilon(\pi)=0.425\ . \tag{3.4}$$

This value is very close to our result and Nightingale and Blöte's[5] calculation of the energy gap [$\varepsilon(\pi)=0.41$].

Figure 6 shows the structure factor $S(q)$. In the case of $S=\frac{1}{2}$, $S(q)$ diverges logarithmically at $q=\pi$. But for the $S=1$ case, it has a Lorentzian-type peak at $q=\pi$,

$$S(q)\propto\{(q-\pi)^2+\xi^{-2}\}^{-1/2}\ . \tag{3.5}$$

In Fig. 7 we show $S(\pi)$ as a function of N. We find that $S(\pi)$ tends to a constant in the limit of $N\to\infty$,

$$S(\pi)\to 3.9\quad (N\to\infty)\ . \tag{3.6}$$

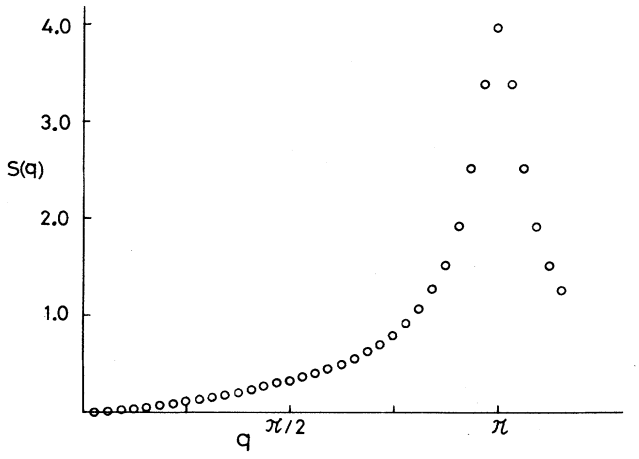

FIG. 6. Structure factor $S(q)$ as a function of q.

IV. CONCLUSION

In this paper we have investigated the spin $S=1$ antiferromagnetic Heisenberg model. We used the large-cluster decomposition Monte Carlo method. We find that the correlation function decays almost exponentially. More precisely, correlation functions are well described with the $2-d$ classical Orstein-Zernike form, that is, the modified Bessel function. Our results support Haldane's conjecture.

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[1]F. D. M. Haldane, Phys. Rev. Lett. **50**, 1153 (1983); Phys. Lett. **93A**, 464 (1983).
[2]R. Botet and R. Jullien, Phys. Rev. B **27**, 613 (1983); R. Botet, R. Jullien, and K. Kolb, *ibid.* **28**, 3914 (1983); M. Kolb, R. Botet, and R. Jullien, J. Phys. A **16**, L673 (1983).
[3]J. C. Bonner and G. Müller, Phys. Rev. B **29**, 5216 (1984).
[4]J. Sólyom and T. A. L. Ziman, Phys. Rev. B **30**, 3980 (1984).
[5]M. P. Nightingale and H. W. Blöte, Phys. Rev. B **33**, 659 (1986).
[6]A. Moreo, Phys. Rev. B **35**, 8562 (1987).
[7]Y. Natsume and M. Matsushita (unpublished).
[8]S. Takada, in *Quantum Monte Carlo Methods,* Vol. 74 of *Springer Series in Solid State Sciences,* edited by M. Suzuki (Springer-Verlag, Heidelberg, 1986), p. 86; K. Kubo and S. Takada, J. Phys. Soc. Jpn. **55**, 438 (1986).
[9]K. Sogo and M. Uchinami, J. Phys. A **19**, 493 (1986).
[10]M. Takahashi, Phys. Rev. B **38**, 5188 (1988).
[11]M. Uchinami, Phys. Lett. A **127**, 151 (1988).
[12]M. Barma and B. S. Shastry, Phys. Lett. **61A**, 15 (1977); Phys. Rev. B **18**, 3351 (1978); J. E. Hirsh, R. L. Sugar, D. J. Scalapino, and R. Blankenbecler, *ibid.* **26**, 5033 (1982).
[13]T. Tsuzuki, Prog. Theor. Phys. **73**, 1352 (1985); **75**, 225 (1986); H. Betsuyaku, *ibid.* **75**, 774 (1986); Y. Okabe and M. Kikuchi, J. Phys. Soc. Jpn. **56**, 1963 (1987); K. Nomura and M. Takahashi, *ibid.* **57**, 1424 (1988).
[14]A. Wiesler, Phys. Lett. **89A**, 359 (1982).
[15]M. Suzuki, Prog. Theor. Phys. **56**, 1454 (1976); J. Stat. Phys. **43**, 886 (1986).
[16]R. M. Fye, Phys. Rev. B **33**, 6271 (1986); M. Suzuki, Phys. Lett. **113A**, 299 (1985).
[17]J. B. Parkinson and J. C. Bonner, Phys. Rev. B **32**, 4703 (1985).
[18]M. Takahashi, Phys. Rev. Lett. **62**, 2313 (1989).