Effects of edges in $S=1$ Heisenberg antiferromagnetic chains

Seiji Miyashita
Graduate School of Human and Environmental Studies, Kyoto University, Kyoto 606, Japan

Shoji Yamamoto
Department of Physics, Faculty of Science, Kyoto University, Kyoto 606, Japan
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Properties of the ground state of open chains of the $S=1$ Heisenberg antiferromagnet are studied by a quantum Monte Carlo method. Size (length) dependences of the ground-state energy, the energy gap, the staggered magnetization $\langle S_i^z \rangle$ and the spin-correlation function $\langle S_1^z S_i^z \rangle$ are investigated under free, fixed, and periodic boundary conditions. The size dependences are significant in chains with less than 25 spins, where the magnitude of the staggered magnetization is rather large. However, the fourfold degeneracy of the ground state and the exponential decay of correlations that are inherent to the Haldane system are recovered when the chain length becomes long enough. Both the staggered magnetization and the spin-correlation function decay exponentially. The correlation length is about six in lattice spacing, which agrees with the value obtained in the bulk.

I. INTRODUCTION

After Haldane's prediction,[1] the low-temperature properties of the $S=1$ Heisenberg antiferromagnetic chain,

$$\mathcal{H}=J\sum_i \mathbf{S}_i\cdot\mathbf{S}_{i+1}\ , \tag{1}$$

have attracted much attention. Detailed numerical investigations have been done especially to make clear both whether a gap exists between the ground state and the first excited state and how the spin-correlation function decays. The existence of the gap was found in fact by a diagonalization method, a transfer-matrix method, and also by various kinds of Monte Carlo methods.[2,3] The spin-correlation function has been investigated mainly by a Monte Carlo method[4] and has turned out to decay exponentially. Effects of an external field have been also studied by a diagonalization method.[5] On the other hand, various analytical approaches have been also tried to clarify the mechanism of these phenomena. In particular, Affleck, Kennedy, Lieb, and Tasaki[6] (AKLT) introduced an exact solvable model which has the typical natures predicted by Haldane and clarified the underlying physical mechanism of the phenomena. Not only the existence of gap, but also the physical origin of the gap has been studied. Affleck and Lieb clarified the difference between the systems with integer spins and those with half-odd-integer spins.[7] Peculiar properties of the ground state have been also discussed. In particular, as an inherent order in the ground-state wave function of the model, the antiferromagnetic alignment of $+1$ and -1, where several zeros are inserted in between them, has been pointed out[8] and the hidden symmetry of the model has been investigated.[9] The characteristics of the wave function of the AKLT-type model have been also discussed based on a factorized wave function.[10] Concerning the nature of the ground state of the system with the free boundary condition, fourfold degeneracy of the ground state and appearance of $S=\frac{1}{2}$ moments at edges have been found in the AKLT model.[6] Kennedy[11] has pointed out that this property of the ground state is also found in a certain kind of model including the pure Heisenberg model (1). The present paper confirms Kennedy's results in long chains using a quantum Monte Carlo method. As to the $S=\frac{1}{2}$ moments at edges, we visualize the local magnetizations and show how a half magnetization appears in the present model with $S=1$.

The existence of the gap has been also confirmed experimentally.[12,13] It was found that $S=\frac{1}{2}$ moment appears[14] at edges of $S=1$ open chains separated by magnetic Cu ions with $S=\frac{1}{2}$ and also by nonmagnetic Zn ions. The effect of edges in open spin chains was also studied by Schwinger-boson mean-field theory.[15]

Recently, Kaburagi, Harada, and Tonegawa have also studied effects of boundary conditions on the energy levels of the Hamiltonian (1) by a diagonalization method.[16] They studied the low-lying energy levels, changing the coupling constant J' between ends of a chain, $\mathbf{S}_1$ and $\mathbf{S}_L$, where L is the chain length. Besides the J' dependence of the energy levels, Kaburagi found that the staggered magnetization is strongly enhanced in finite open chains with odd numbers of spins and the wave function for $M_z=\pm 1$ is qualitatively very much different from that for $M_z=0$.[17] The data for an open chain with 13 spins show a very long correlation, which raises the question of whether the boundary condition changes the bulk property. However, in the AKLT model, the bulk properties do not depend on the boundary condition and the effect of a boundary decays in the same way in the bulk correlation, i.e., as $(-3)^{-r}$, where r is the distance. In particular, in the ground state of the system with finite length L with $M_z=1$, local magnetic moments distribute as[18]

$$\langle S_j^z \rangle = (-)^j \frac{2}{\sqrt{3}} \begin{cases} \sinh\left[\dfrac{j-(L+1)/2}{\xi}\right] \Big/ \sinh\left[\dfrac{L}{2\xi}\right] & (L=\text{even}) \\ -\cosh\left[\dfrac{j-(L+1)/2}{\xi}\right] \Big/ \cosh\left[\dfrac{L}{2\xi}\right] & (L=\text{odd}) , \end{cases} \tag{2}$$

where $\xi = 1/\ln 3$. In the present model, the correlation length in the bulk has been found to be about 6.2 in lattice spacing, which was estimated in a system with the periodic boundary condition.[4] In this circumstance, we study the size (length) dependence of spatial distribution of the staggered magnetic moments and the correlation functions in the present model. We employ a quantum Monte Carlo method based on the Suzuki-Trotter decomposition. In order to clarify effects of the edge, we investigate open chains of two types. One has free boundaries at both ends and the other has a fixed spin at an end. For each chain, we consider both cases of odd and even numbers of spins. For comparison we also carry out calculations in the case of the periodic boundary condition. In chains with odd numbers of spins (odd chains), the ground state is in the space of S (the total spin) $=1$. In the cases of $M_z = \pm 1$, the system has a finite static staggered magnetization ($\mathcal{N}_z$)

$$\mathcal{N}_z = \sum_{j=1}^{L} (-1)^j S_j^z . \tag{3}$$

In finite odd chains, we find a rather large staggered magnetization as Kaburagi has found. On the other hand, $\mathcal{N}_z$ is zero in the subspace of $M_z = 0$ in $S=1$. In the ground state of chains with even numbers of spins (even chains), the total spin is zero ($S=0$) and consequently $\mathcal{N}_z$ does not appear, either. If we fix a spin at an end, we find that $\mathcal{N}_z$ is enhanced in odd chains and it appears even in even chains. In both cases, however, we have found that the staggered magnetization decays exponentially with the same correlation length in the bulk when the length of the chains become long enough.

Because the magnetization $M_z = \sum_j S_j^z$ commutes with the Hamiltonian in the present model (1), the ground state must not be changed by a magnetic field less than a critical value at which the energies of the ground state and a state with nonzero magnetization cross. In an odd chain, the ground state is a triplet and has the threefold degeneracy which is lifted up by a magnetic field. Therefore, natures of the ground state may be affected even by a field below the critical field. Since the staggered moments are large in the ground states of short odd chains, it is expected that local staggered moments are observed in real materials which consist of open chains with various length. Some experimental results suggest such an effect.[19]

In Sec. II we explain the model and method. We give in Sec. III the size dependences of the staggered moments, the spin-correlation functions, and the ground-state energy. Section IV is devoted to summary and discussion.

II. MODEL AND METHOD

In this paper we study the model (1) without a magnetic field by a quantum Monte Carlo method based on the Suzuki-Trotter decomposition.[20] Here we use the so-called checkerboard decomposition[21]

$$e^{-\beta\mathcal{H}} \to (e^{-\beta\mathcal{H}_A/n} e^{-\beta\mathcal{H}_B/n})^n , \tag{4}$$

where $\beta = (k_B T)^{-1}$ and

$$\mathcal{H}_A = J \sum_{i=1,3,\ldots} \mathbf{S}_i \cdot \mathbf{S}_{i+1}, \quad \mathcal{H}_B = J \sum_{i=2,4,\ldots} \mathbf{S}_i \cdot \mathbf{S}_{i+1} . \tag{5}$$

Simulations are performed on a transformed two-dimensional $S=1$ Ising system with four-body interactions representing the local Boltzmann factor [Fig. 1(a)],

$$\rho(S_i, S_{i+1}, S_i', S_{i+1}') = \langle S_i, S_{i+1} | e^{(\beta J/n)\mathbf{S}_i \cdot \mathbf{S}_{i+1}} | S_i', S_{i+1}' \rangle . \tag{6}$$

Here S_i takes ± 1 and 0. The algorithm of simulation is quite similar to the case of $S=\frac{1}{2}$. A flip procedure in this case is, however, a little more complicated than the case of $S=\frac{1}{2}$. Besides the local flips of exchange type [Fig. 1(b)], which are used in the case of $S=\frac{1}{2}$, the local flips shown in Fig. 1(c) should be taken into account. Because of the free boundary condition, there is no difficulty in simulations concerning to the ergodicity of the winding number.[22] Because of the conservation law of the magnetization in a plaquette shown in Fig. 1(a)

$$S_i + S_{i+1} = S_i' + S_{i+1}' , \tag{7}$$

the state of the plaquette can be specified by only three

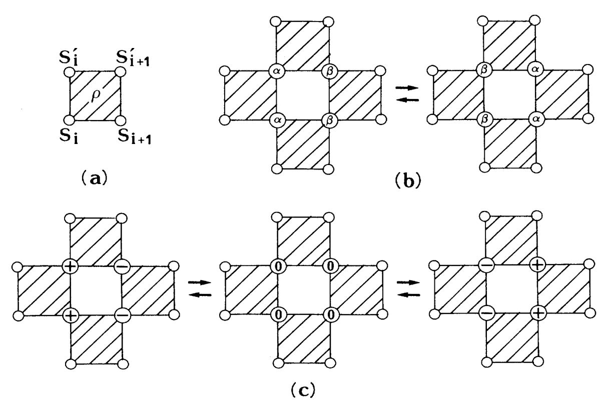

FIG. 1. (a) Plaquette with the four-body interaction. (b) Local flip of exchange type. (c) Local flip in the cases of $S=1$.

TABLE I. The lowest energies for $M_z=0$ and 1.

L		13(12)		25(24)		33(32)		65(64)	
M_z		0	1	0	1	0	1	0	1
A	EX5	−17.13	−17.15	−34.07	−34.07	−45.38	−45.37	−90.57	−90.58
	EX4	−17.05	−17.07	−33.91	−33.91	−45.16	−45.16	−90.14	−90.13
	EX3	−17.02	−17.05	−33.85	−33.86	−45.09	−45.08	−89.97	−89.98
B	EX5	−15.77	−15.68	−32.67	−32.66	−43.96	−43.96	−89.17	−89.18
	EX4	−15.69	−15.61	−32.51	−32.51	−43.75	−43.76	−88.73	−88.73
	EX3	−15.68	−15.59	−32.45	−32.46	−43.68	−43.69	−88.58	−88.59
C	EX5	−16.98	−16.49	−33.91	−33.47	−45.21	−44.77	−90.41	−89.97
	EX4	−16.90	−16.41	−33.74	−33.29	−44.98	−44.53	−89.95	−89.51
	EX3	−16.88	−16.38	−33.68	−33.22	−44.89	−44.44	−89.81	−89.34
D	EX5	−16.27	−16.79	−33.16	−33.70	−44.47	−45.00	−89.66	−90.20
	EX4	−16.08	−16.66	−32.90	−33.49	−44.14	−44.73	−89.11	−89.71
	EX3	−15.98	−16.60	−32.77	−33.39	−43.99	−44.62	−88.88	−89.53
E	EX5	−14.82	−15.28	−31.74	−32.29	−43.05	−43.59	−88.25	−88.79
	EX4	−14.64	−15.16	−31.48	−32.08	−42.72	−43.32	−87.70	−88.30
	EX3	−14.55	−15.10	−31.35	−31.99	−42.57	−43.19	−87.47	−88.13

spins of them. Thus, we label states of each plaquette by a code number from 0 to 26 $[9(S_i+1)+3(S_{i+1}+1)+S_i'+1]$. In most cases, we performed 10^5 Monte Carlo steps (MCS) and the first 2×10^4 MCS were discarded as the initial transient stage. We use the Trotter number n in the range $8\le n\le 48$ and the n dependence is extrapolated by the least-squares method using the formula

$$A(n)=A_\infty+\frac{A_1}{n^2}+\frac{A_2}{n^4}\ . \tag{8}$$

The results depend on the ways of extrapolation. Then we list the results obtained by three different extrapolations. One uses the data for $n=12$, 16, 24, 32, and 48, one uses the data for $n=16$, 24, 32, and 48 and the other uses the data for $n=24$, 32, and 48. They are denoted by EX5, EX4, and EX3. Comparing with known data, EX3 seems to give the best values. The difference between values by EX3 and EX4 is considered to give the order of ambiguity. The precision of the data is about three digits and it may be not quite enough to investigate the value itself. But it is enough to study the size dependences of the values. In order to study the size dependences of the magnetization profiles and the spin-correlation functions, the present precision is good enough as shown in the following sections. An example of the extrapolation is shown in Appendix. The values of the energy E, the staggered magnetization $\langle \mathcal{N}_z\rangle$ and the square of the staggered magnetization $\langle \mathcal{N}_z^2\rangle$ are listed in Tables I, II, and III, respectively, where A and B represent open odd and even chains with free boundaries at both ends. C represents periodic chains and D and E represent open odd and even chains with a fixed spin at an end.

In order to check the validity of our method, in the case of $L=5$, we have compared our Monte Carlo data for each n with the exact values obtained by a transfer-matrix method. We also confirmed the extrapolated data in the case of $L=13$ agree with the values obtained by an exact diagonalization method.

The global flip to change the value of M_z, namely the flip along the Trotter axis, is not used because we study the M_z dependence of the nature of the ground state. We have carried out simulations at temperatures $\beta^{-1}\equiv k_BT=0.05$ and 0.1. In both cases almost the same extrapolated values have been obtained. Thus we regard $\beta^{-1}=0.05$ to be small enough to obtain the ground-state properties. The temperature dependence of the data will be published elsewhere, where the above-mentioned global flip must be included.

In simulations for the periodic chains the global flips are necessary to recover the ergodicity of the winding number. But the data obtained for $L=12$ without the global flips seem to agree with the exact data.[17] The data also agree with the previously obtained data.[4] Thus we have here obtained data by simulations without the global flips. Detailed analysis of the dependence on the global flips will be reported elsewhere.

III. RESULTS

A. The staggered magnetization

As Kaburagi has pointed out, in finite odd chains the staggered magnetization appears in the ground state with

TABLE II. The staggered magnetization in the case of $M_z=1$.

L		13	25	33	65
A	EX5	5.00	5.91	6.27	6.52
	EX4	5.00	5.96	6.32	6.21
	EX3	4.99	5.86	6.50	7.14
D	EX5	6.99	8.63	8.84	9.08
	EX4	6.96	8.61	9.22	9.32
	EX3	6.87	8.56	9.26	9.86
E	EX5	2.52	2.56	2.89	3.04
	EX4	2.51	2.60	2.64	2.94
	EX3	2.45	2.43	2.63	2.26

TABLE III. The square of the staggered magnetization.

L		13(12)		25(24)		33(32)		65(64)	
M_z		0	1	0	1	0	1	0	1
A	EX5	27.08	48.80	68.60	101.18	98.81	135.50	220.35	265.21
	EX4	27.01	48.60	68.72	102.50	97.65	136.65	215.50	257.41
	EX3	27.15	48.46	68.43	102.54	97.84	138.94	221.10	279.65
B	EX5	41.38	24.33	97.47	65.25	135.20	94.25	253.68	216.11
	EX4	41.29	24.18	99.47	65.86	133.72	94.92	254.04	217.20
	EX3	41.20	24.16	100.78	66.55	134.71	95.67	251.65	213.14
C	EX5	40.95	25.38	89.12	67.74	120.30	98.01	243.16	221.07
	EX4	40.94	25.27	90.30	67.41	121.42	98.19	239.03	219.65
	EX3	40.77	25.07	88.41	66.50	120.41	97.46	252.54	222.82
D	EX5	39.94	66.25	97.06	131.22	127.53	165.02	254.35	295.06
	EX4	39.88	66.03	99.17	131.68	128.58	173.37	258.24	296.65
	EX3	40.39	65.14	100.12	129.45	134.92	174.49	266.21	304.28
E	EX5	21.02	25.28	61.54	63.56	91.22	94.82	216.10	217.74
	EX4	20.95	25.25	61.73	63.91	91.21	93.23	209.62	216.10
	EX3	20.77	24.98	61.73	62.34	89.81	90.64	206.18	214.12

$M_z=\pm1$. In Fig. 2(a) the magnetizations $\langle S_i^z\rangle$ ($i=1,\ldots,L$) in the ground state with $M_z=1$ are plotted for $L=13$, 25, and 33. The longer the chain length, the faster the staggered magnetization decays. Data for $L=65$ and 97 are also given in Fig. 2(b), where we find that the end magnetizations decay almost in the same way. Here we can clearly see that one half of the total magnetization ($M_z=1$) is localized in each end as has been known in the AKLT model. The data are also plotted in logarithmic scale in Fig. 3. In long chains the moments decay exponentially

$$\langle S_j^z\rangle \propto e^{-j/\xi} . \tag{9}$$

Here we have estimated $\xi\sim6$, which is consistent with the value estimated in the periodic chains.[4] However, it should be noted that the minimum moment $\langle S_i^z\rangle$ is about 0.10 even for $L=33$, which is rather large.

If we fit the present data taking into account the finite-size effect, namely in the form, $\langle S_j^z\rangle \propto e^{-(j-1)/\xi} + e^{-(L-j)/\xi}$, we find that $\xi\sim6$ is consistent even for $L=13$, although its slope in Fig. 3 looks much gentler.

Next, we fix a spin at an end. In Fig. 4(a), data for $L=13$, 25, 33, and 65 are plotted, where we find that the staggered moments on the side with the fixed spin are enhanced but no effect is seen on the other side. If we fix a spin at an end in even chains, the magnetizations are induced but they show a complicated profile. In Fig. 4(b) data for $L=12$, 24, and 32 are plotted. We find again that the magnetization decays exponentially with the same correlation length.

With these observations, we conclude as follows. The finite-size effect is significant for $L\le25$. On the other hand, in longer chains the effect of edge decays exponentially and the correlation length is the same as that in the

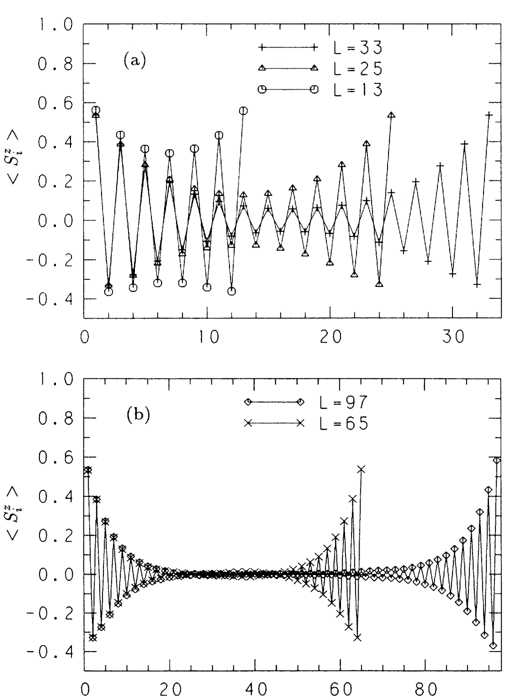

FIG. 2. (a) The staggered magnetic moments $\langle S_i^z\rangle$ in chains with free boundaries at both ends in the cases of $L=13$, 25, and 33. (b) The staggered magnetic moments $\langle S_i^z\rangle$ in chains with free boundaries at both ends in the cases of $L=65$ and 97.

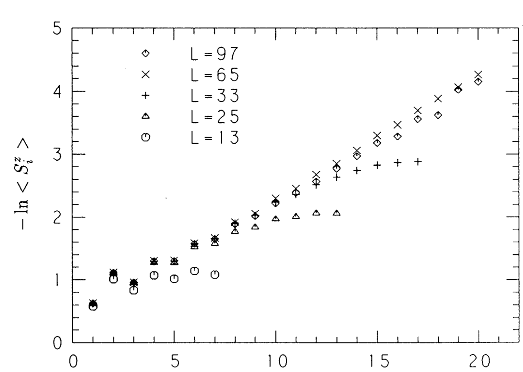

FIG. 3. Logarithmic plot of the staggered magnetic moments shown in Fig. 2.

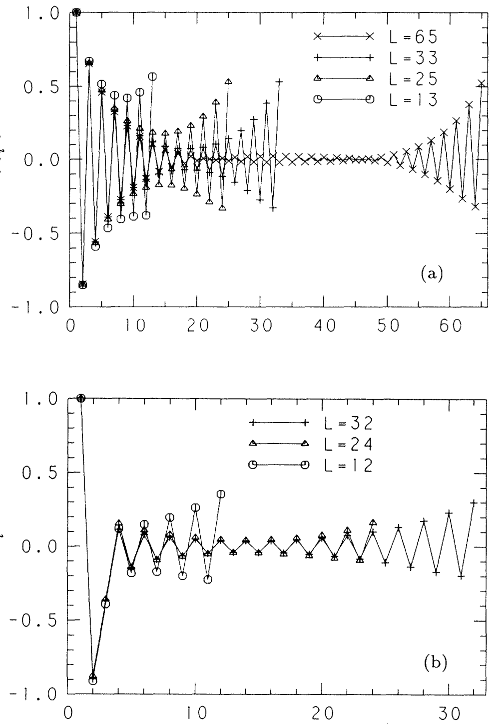

FIG. 4. (a) The staggered magnetic moments $\langle S_i^z \rangle$ in chains with a fixed spin at an end in the cases of $L=13$, 25, 33, and 65. (b) The staggered magnetic moments $\langle S_i^z \rangle$ in chains with a fixed spin at an end in the cases of $L=12$, 24, and 32.

bulk, as is known for the AKLT model. The total staggered magnetization $\mathcal{N}_z$ are listed in Table II.

B. The spin-correlation functions

We have also studied the spin-correlation function between S_1^z and S_i^z, $\langle S_1^z S_i^z \rangle$. It remains finite even in the ground state of even chains and periodic chains, while the moment itself $\langle S_i^z \rangle$ vanishes in these chains. Then, in this section, the correlation functions are investigated for all types of chains. But the cases of chains with a fixed spin $S_1=1$ are not considered because $\langle S_1^z S_i^z \rangle = \langle S_i^z \rangle$. The data are plotted in Fig. 5 for odd chains with $M_z=1$ (a), for even chains with $M_z=0$ (b) and for periodic chains with $M_z=0$ (c). The data shown in Fig. 5(a) are also plotted in logarithmic scale in Fig. 6 and we find again the exponential decay with almost the same correlation length observed in Fig. 3. In the case of odd chains with $M_z=0$ and also of even chains with $M_z=1$, similar correlation functions are found but a node is found at the center of the chain due to the geometrical restriction. In other words, there exists a domain wall in the Néel order. We list in Table III the square of the total staggered magnetization, which is the summation of all the staggered spin-correlation function,

$$\langle \mathcal{N}_z^2 \rangle = (1/L) \sum_{ij} (-1)^{i+j} \langle S_i^z S_j^z \rangle \ .$$

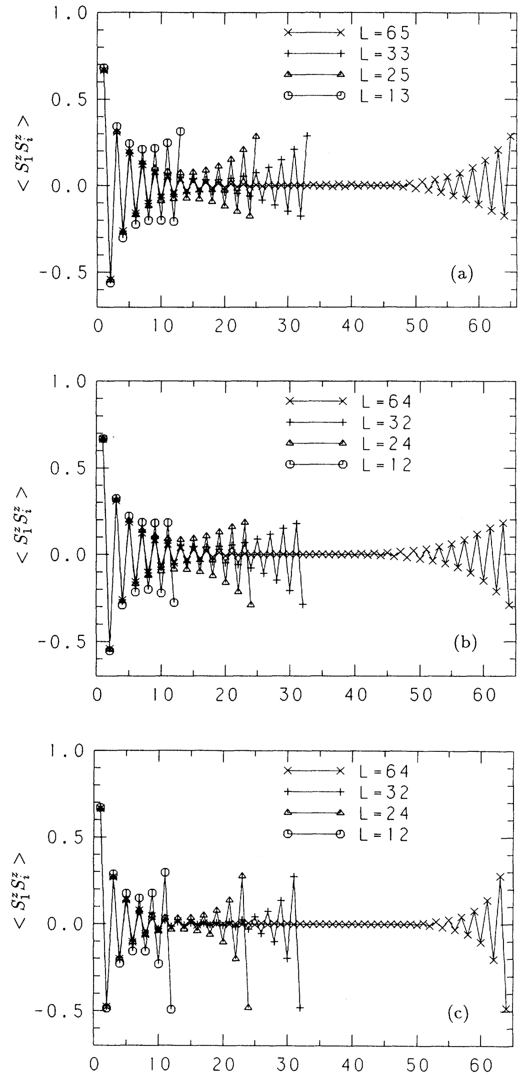

FIG. 5. (a) The correlation functions $\langle S_1^z S_i^z \rangle$ in odd chains in the case of $M_z=1$. (b) The correlation functions $\langle S_1^z S_i^z \rangle$ in even chains in the case of $M_z=0$. (c) The correlation functions $\langle S_1^z S_i^z \rangle$ in periodic chains in the case of $M_z=0$.

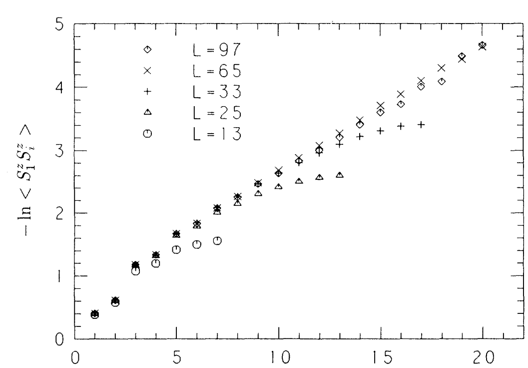

FIG. 6. Logarithmic plot of the correlation functions shown in Fig. 5(a).

TABLE IV. Size dependences of the lowest energies for $M_z=0$ and 1.

L	8		12		16		20	
M_z	0	1	0	1	0	1	0	1
EX5	−10.18	−9.98	−15.77	−15.68	−21.38	−21.35	−27.02	−27.01
EX4	−10.14	−9.94	−15.69	−15.61	−21.28	−21.25	−26.89	−26.88
EX3	−10.13	−9.93	−15.68	−15.59	−21.26	−21.22	−26.86	−26.84
ΔE^a	0.2		0.09		0.04		0.02	
$\Delta E^b_{\text{exact}}$	0.2019		0.0971		0.0496			

[a]The gap between the energies for $M_z=0$ and 1 evaluated with the data EX3.
[b]Energy gaps obtained by a diagonalization method (Ref. 23).

C. The ground-state energy

Let us consider the size dependence of the energy structure. For free odd chains, the ground state is in the subspace of $S=1$ and has threefold degeneracy with $M_z=\pm1$ and 0. Thus the lowest energies in the subspaces with $M_z=1$ and 0 should be the same. On the other hand, for free even chains, the ground state is singlet ($S=0$) and the lowest energy state with $M_z=1$ gives the first excited state with $S=1$. This is true for chains with the free boundary condition as well as for ones with the periodic boundary condition. But reflecting the fourfold degeneracy in open chains, which is inherent to the Haldane problem, in open free chains the gap becomes small as the chain length becomes long while the gap remains finite in the periodic chains, as Kennedy has pointed out.[11] In order to study the size dependence of the gap, we have also performed Monte Carlo simulations for $L=8$, 16, and 20. The size dependence is given in Table IV. If we assume an exponential dependence of the gap on L, $\Delta E \sim e^{-r/\xi_E}$, we find ξ_E is about 5.3, which is close to the correlation length of the spin-correlation function. This observation seems not compatible with the prediction, $\xi_E \geq 2\xi$, in Ref. 15.

IV. SUMMARY AND DISCUSSION

Finite-size effects in open chains have been investigated by a quantum Monte Carlo method. It has been found that the edge effect decays exponentially with the correlation length, which is the same as that in the bulk. In short odd chains, however, rather large magnetic moments are observed. If we fix a spin at an end, the staggered moments are enhanced. Since the fixed spin causes staggered magnetization nearby, some pinning effects of spins cause local staggered orders. The Néel orders thus induced appear only locally and they do not make a consistent long-range Néel order. However, they cause a static field on atoms near the impurity.

Let us consider the field dependence of such a local order. A system may have a small perturbation V which does not commute with M_z, such as $E_{xy}=(S_i^x)^2-(S_i^y)^2$. Then the threefold degenerate ground state of open odd chains become no more diagonal to each other and they would be exchanged and the staggered magnetization would be averaged out to vanish. On the other hand, in a field, a state with the favorable magnetization is selected as the ground state and the local staggered moments $\langle S_i^z\rangle$ are stabilized against the perturbation V. In the present mechanism, the local staggered order should be parallel to the field in contrast to the case of the classical system where the staggered moments are perpendicular to the field (Fig. 7). In the real materials there exist many perturbations and some of them may take the role of the above-mentioned perturbations. We hope that the present mechanism of appearance of a local staggered field would be observed experimentally, for example, in the NMR or electron spin resonance experiments, which are sensitive to the existence of a static internal field even when the field is not uniform in the system.

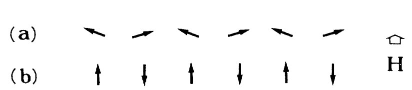

FIG. 7. (a) Schematic field dependence of the orientation of spins in classical systems. (b) Schematic field dependence of the orientation of spins in the present mechanism.

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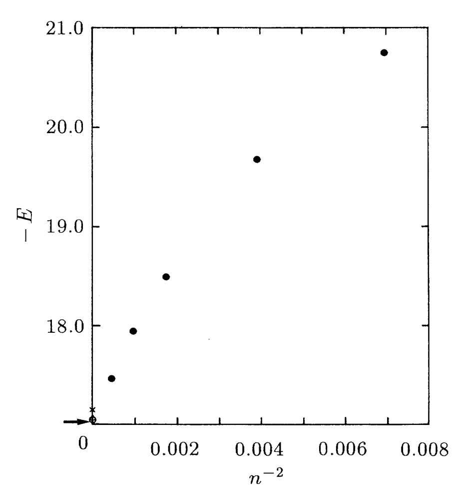

FIG. 8. Dependence of the energy of $L=13$ open free chain on the Trotter n and the extrapolated points by EX5 (×), by EX4 (△) and by EX3 (○). The exact value is indicated by an arrow.

formed from TITPACK of Nishimori for $S=\frac{1}{2}$. They also thank Professor H.-J. Mikeska and Dr. T. Sakai for valuable discussions. Numerical calculations were performed on FACOM VP2600 of Kyoto University. This work is partially supported by a Grant-in-Aid for Scientific Research on Priority Areas, Computational Physics as a New Frontier in Condensed Matter Research, from Ministry of Education, Science and Culture.

APPENDIX: THE EXTRAPOLATION $n \rightarrow \infty$

Here we demonstrate how the data are extrapolated with the form of (8). For the free odd chain with $L=13$, the obtained values of the energy in the unit J at $T=0.05$ are 20.741, 19.685, 18.502, 17.937, and 17.468 for $n=12$, 16, 24, 32, and 48, respectively. The error bar of the data is about 0.01. The exact ground-state energy is 17.028. The extrapolations, EX5, EX4, and EX3 give the values, $E_5=17.15$, $E_4=17.07$, and $E_3=17.05$. The data are plotted in Fig. 8. As is suggested by this example, this extrapolation ($n \rightarrow \infty$) has rather large ambiguity. In the present case, the larger the n, the more significant the bending of the n dependence becomes. Therefore, EX3 gives the best estimation and EX4 gives a slightly larger estimate caused by the data with smaller n's. EX5 gives a rather large estimate. Generally, EX4 and EX3 seem to give reliable values and the difference between them can be regarded as the order of ambiguity of the estimations.

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