Boundary effects in the density-matrix renormalization group calculation

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We investigate *the boundary effect* of the density matrix renormalization group calculation (DMRG), which is an artifactual induction of symmetry-breaking pseudo-long-range order and takes place when the long-range quantum fluctuation cannot be properly included in the variational wave function due to numerical limitation. The open boundary condition often used in DMRG suffers from the boundary effect the most severely, which is directly reflected in the distinct spatial modulations of the local physical quantity. By contrast, the other boundary conditions such as the periodic one or the $\sin^2$-deformed interaction [A. Gendiar, R. Krcmar, and T. Nishino, Prog. Theor. Phys. **122**, 953 (2009)] keep spatial homogeneity, and are relatively free from the boundary effect. By comparing the numerical results of those various boundary conditions, we show that the open boundary condition sometimes gives unreliable results even after the finite-size scaling. We conclude that the examination of the boundary condition dependence is required besides the usual treatment based on the system size or accuracy dependence in cases where the long-range quantum fluctuation is important.

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I. INTRODUCTION

The density matrix renormalization group (DMRG) proposed by White[1] is by now one of the most powerful numerical tools to determine the ground states and low-energy excitations[2,3] of the correlated quantum many-body systems in low dimensions. Accumulated studies revealed that the DMRG has advantages when the system is not critical (gapped), where one could effectively reduce the number of basis states without sacrificing the numerical accuracy. The open boundary condition (OBC) usually used in the DMRG analysis also works to reduce the number of bases, which was pointed out by White in the first stage.[1] In fact, compared to the periodic boundary condition (PBC), OBC has a smaller number of joint points between the blocks (subsystems) than PBC (one and two points, respectively), and thus has smaller entanglement entropy which follows a concept of area law:[4] the smaller the size of the boundary between the two blocks, the smaller the entanglement entropy one finds between them. However, one shall have to be careful in this context because the existence of the open edge points does not only indicate the reduced entanglement, but means the breaking of the translational symmetry which leads to two artifacts in critical (gapless) systems. One is to favor a particular fraction of ground-state manifolds which are equivalently degenerate in the bulk limit. The other is *to mix partially the states which have different symmetric properties from the ground-state manifold*. The former effect does not modify the ground-state nature (only chooses a pure state) and is equivalent to introducing the infinitesimal symmetry-breaking field in large systems (see Sec. II A for details). However, the latter may sometimes allow some low-energy excited state to overwhelm the original ground state. For example, when the correlation length is longer than the typical system size, the oscillation induced by the open boundary may open an apparent gap, particularly when the number of states kept is not large enough. This is what we call the "boundary effect."

The portion of boundary is order 1 while the system is order L, and by the finite-size scaling, the boundary effect is expected to decay faster than $1/L$ on an average. Therefore, by the proper finite-size scaling, one could in principle get rid of the boundary effect, and the correlation with the largest length scale is considered to be the one characterizing the ground state. In fact, one can take advantage of the OBC in order to examine the nature of orders or correlations: Due to the boundary edges, the wave function loses the translational symmetry, and the two-point correlation of the largest length scale explicitly appears as a spatial modulation of *local physical quantities*. This treatment was actually applied to DMRG by the present authors. In the one-dimensional Kondo lattice model (KLM) the two open edges are regarded as impurities which induce the Friedel oscillations, and by measuring the structural factors of the charge or spin amplitudes, the authors detected the wave numbers, $2k_F$ or $4k_F$, of the Tomonaga-Luttinger liquid state.[5] Also in two dimensions, the competition of several different types of long-range orders with different spatial periodicity is detected by the spatial modulation of particle density in the fermionic model on an anisotropic triangular lattice under the chemical potential on system edges.[6] Such analysis is, however, applicable only when the basic nature of the ground state is already understood; namely, it *clarifies the details of the already known (stable) ground state but not the ground state itself*. Moreover, the analysis requires a set of results with high enough accuracy as well as a parameter region where the scaling law is safely adopted. Once either of the above two is not fulfilled, one may no longer obtain a reliable result, which is often the case in DMRG, since there is an upper bound of the number of states kept, in practice.

The present paper discusses how to classify systematically the state which does or does not break any symmetry of the original Hamiltonian within a usual numerical accuracy of DMRG. We examine how the critical behavior of quantum many-body states at finite system size is influenced by the boundary condition by choosing two characteristic examples: a well-known symmetry-broken long-range order in a spin chain, and strongly correlated electronic states with extremely long correlation length. We consider the modified or deformed OBC, as well as PBC, and demonstrate that the expectation

value of the local operator depends severely on boundary conditions so that they cannot be a reliable measure. We finally see that in order to conclude the presence of long-range order, it is necessary to confirm that *the two-point correlations remain finite toward the bulk limit irrespective of the boundary conditions*.

II. BOUNDARY CONDITIONS

A. Symmetry-breaking long-range orders

We consider a class of long-range orders due to translational symmetry breaking; i.e., the order operators do not commute with the quantum Hamiltonian of crystals which usually keeps the translational symmetry. It is known that even when such spontaneous symmetry breaking occurs in the bulk limit, quantum fluctuation "obscures" the breaking of symmetry at finite system size and one finds a unique ground state with perfect symmetry.[7,8]

Let us briefly follow the contexts of Ref. 7 by Koma and Tasaki, which is based on two different kinds of measures,

$$m_s = \lim_{B\to 0}\lim_{L\to\infty} m_s(B,L),$$
$$m_s(B,L) = \frac{1}{L}\left\langle \sum_i O_i(B,L)\right\rangle, \tag{1}$$
$$\sigma = \lim_{L\to\infty}\sigma(L),$$
$$\sigma(L) = \frac{1}{L}\sqrt{\left\langle\left[\sum_i O_i(B=0,L)\right]^2\right\rangle}, \tag{2}$$

where $\langle O_i(B,L)\rangle$ is the expectation value (trace) of local operator $O_i(B,L)$ on the ith site under the symmetry-breaking field B and for system size L. Hereafter, we use mere O_i as the one with $B=0$ and finite L except otherwise noted. In the Heisenberg antiferromagnet, m_s is the staggered magnetization obtained by applying the infinitesimally small symmetry-breaking field, $B\to 0$, whereas the latter is the conventional long-range order parameter which consists of two-point correlation functions, $\langle O_i O_j\rangle$, between sites i and j. Koma and Tasaki proved that

$$m_s \geqslant r\sigma \tag{3}$$

holds for constant r at all temperature for various types of models with long-range order [$r=1$ holds in general, but a higher symmetry gives stronger bounds, e.g., $r=\sqrt{3}$ for the SU(2) Heisenberg antiferromagnet[7,9]]. Here, $\sigma>0$ means that the two-point correlation function does not decay to zero in the bulk limit, $\langle O_i O_j\rangle \neq 0$ for $|i-j|\to\infty$. Therefore, Eq. (3) indicates that $\sigma>0$ guarantees the existence of symmetry breaking represented by $m_s>0$.

We now interpret Eq. (3) to the numerical analysis on a finite-size system at zero temperature. Note that the following Eqs. (4)–(7) and conditions (I)–(III) are conjectures, which are derived logically in the following part of this section. Since the finiteness of the system is characterized by the presence of boundaries, we first discuss the role of boundary conditions. When the system does not have any open edges, e.g., periodic (PBC) or antiperiodic (APBC) boundaries, the translational symmetry in the Hamiltonian "obscures" the breaking of translational symmetry at finite L, and we find $\langle O_i(L<\infty)\rangle_{\rm pbc}=0$. Thus we need to include the infinitesimal symmetry-breaking field B, or analyze the two-point correlation function $\sigma(L)_{\rm pbc}$, which coincides with σ in the limit of large L: $\lim_{L\to\infty}\sigma(L)_{\rm pbc}=\sigma$.

In the case of open boundary condition, the coupling between the 1st and the Nth sites in PBC is missing and the translational symmetry is broken in the Hamiltonian. This works to discriminate the two edge bonds energetically from the rest of the bonds in the system, which approximately corresponds to placing the effective external field on the edge bonds.[10] Such effective local field induces oscillation of local correlations, which is absent in PBC.

We basically confine ourselves to the case where the period of the oscillation is compatible with the interval between edge bonds; e.g., if the induced oscillation has twofold periodicity, the number of bonds, $L-1$, must be odd. Then the open boundary condition corresponds to a locally introduced symmetry-breaking "field," $B_{\rm ob}$, which is coupled to the local operator $O_i = o_{i+1}o_{i+2} - o_i o_{i+1}$ at the edge sites, $i=1$ and N, where o_i is the operator acting on the ith site. The effect of $B_{\rm ob}$ decays as it propagates toward the system center from both edges, which is reflected in the gradual decrease of the oscillation amplitude of $\langle O_i\rangle$ with $i\to N/2$. Then, we expect $m_s(L)_{\rm obc}\geqslant m_s$. The two-point correlation functions $\langle O_i O_j\rangle_{\rm obc}$ are those under the effective symmetry breaking "field," so that we shall find $\sigma(L)_{\rm obc}\geqslant\sigma$.

Basically the portion of boundary is order 1 while the system is order L, and taking the limit of $L\to\infty$ corresponds qualitatively to having $B_{\rm ob}\to 0$ as in Eq. (1). Thus both of the above two boundary conditions (PBC and OBC) lead to the same conclusion,

$$m_s = \lim_{B\to 0}\lim_{L\to\infty} m_s(B,L)_{\rm pbc} \tag{4}$$
$$= \lim_{L\to\infty} m_s(B=0,L)_{\rm obc}, \tag{5}$$
$$\sigma = \lim_{L\to\infty}\sigma(L)_{\rm pbc} \tag{6}$$
$$= \lim_{L\to\infty}\sigma(L)_{\rm obc}, \tag{7}$$

with $m_s\geqslant\sigma$. We therefore conclude that when $\sigma>0$, we always find $m_s>0$.

However, the numerical approximation, e.g., restricting the number of basis to m in DMRG, sacrifices the inclusion of long-range quantum fluctuation to some extent. The OBC does not only work as an "effective symmetry-breaking field," but its locality induces a nonuniformity of the quantum fluctuation and mixes the states which have different symmetry from the original pure state. While such additional effects may be weakened as $L\to\infty$, incomplete long-range quantum fluctuations sometimes cause harmful effect on the original ground-state symmetry as we will see shortly. Therefore, the practical procedure to systematically get rid of the artifact of the boundary condition is required.

The above-mentioned nonuniformity under OBC is reflected in $\langle O_i\rangle$ and $\langle O_n O_{n+i}\rangle$, and their deviation from the one in the uniform system is enhanced near the open edges. Since we need to analyze the systematic behavior of these quantities in large systems, we examine them at each site i and n instead of taking their mean value over the whole

system as in Eqs. (1) and (2). Then, those of site i and n away from the edges are adopted which should fulfill $\lim_{L\to\infty}\langle O_i\rangle \gtrsim r \lim_{L\to\infty}\langle O_n O_{n+i}\rangle$ as in Eq. (3).

With this in mind, we propose *the necessary conditions* the numerical results must fulfill in order to safely conclude the breaking of translational symmetry in the bulk limit:

(I) the two-point correlation function $\langle O_n O_{n+i}\rangle$ remains finite for $i \to L/2$, after the L and m scaling,

(II) the conclusion obtained by (I) does not depend on the boundary conditions, including those with and without symmetry breaking,

(III) as $\langle O_i\rangle$ of finite systems becomes uniform under the variation of the boundary conditions, the corresponding two-point correlation function $\langle O_n O_{n+i}\rangle$ approaches the value of the pure state in the bulk limit.

The rest of the paper is devoted to the numerical "proof" of this conjecture or proposal in the representative models in one dimension.

The boundary conditions we consider are classified into those which keep the translational symmetry and those which do not. As a typical boundary condition of the former class, we deal with the system with "deformed interactions" recently proposed by Gendiar, Krcmar, and Nishino,[11] as well as the PBC and APBC. The representative condition of the latter class is the OBC. Besides, we consider the cases referred to as *modified open boundary*, which is the open boundary with potentials on edge sites or edge bonds first adopted by White and Huse.[12] As we discussed in this section, the open boundary works as an effective field on edges, which brings the spacial nonuniformity of the quantum states. This artificial effect can be suppressed by adjusting the bond strength or potentials on edges by hand, and thus one can tune the degree of inhomogeneity by the "modification of the open boundary."

We finally comment on the cases where the period of oscillation of local quantity $\langle O_i\rangle$ does not match the length of the system L. For example, in the case of dimer order, the local operator O_i is defined as $O_i = \boldsymbol{S}_{i+1}\cdot\boldsymbol{S}_{i+2} - \boldsymbol{S}_i\cdot\boldsymbol{S}_{i+1}$, and the twofold periodic oscillation appears in the nearest-neighbor spin-spin correlation. In the odd-L system with PBC, a kink, namely a twisting oscillation, emerges in the system. Since the PBC keeps translational symmetry, the wave function should be the superposition of L different wave functions, each with a kink on the ith ($i = 1 \sim L$) bond. Then, $\langle O_i\rangle$ is uniform but is suppressed from the one without a kink by the order of $1/L$, which recovers the bulk value when $L \to \infty$.

When the system of odd L has an open boundary, this kink is confined to the center site as $\langle O_{L/2}\rangle \sim 0$. This is because the dimer bond is pinned the strongest at both edge bonds, and the oscillations of $\langle O_i\rangle$ starting from these strong edge bonds interfere at the center and form a kink.[13] The effect of this kink on $\langle O_{L/2}\rangle$ cannot be excluded by the m or L scaling, since it is locked at the center of the system. The artifact of kink on the value of $\langle O_n O_{n+i}\rangle$ is also nontrivial, and less easy to get rid of compared to the usual boundary effect of OBC with even L. We show in Sec. IV that $\langle O_n O_{n+i}\rangle$ in the dimer state with a kink in OBC finally approaches the value without a kink with phase shift π, which means that (II) basically holds regardless of the presence or absence of a kink. In this sense we can judge the presence of the dimer order even in the system of odd L with a kink.[14]

In the above semiclassical picture, the kink is localized on a single bond. However, in the quantum systems we deal with, the kink spreads over a certain length scale due to quantum fluctuation, and this length scale depends on the stiffness of the dimer order. Still, if we take L enough larger than this length scale, the same discussion holds.

B. Modified open boundary

The analysis with modified open boundary in DMRG was first adopted in the $S = 1$ Haldane chain with $S = 1/2$ spins on the edge sites by White and Huse.[12] To evaluate the Haldane gap of infinite systems, they adjusted the coupling, $J_{\rm end}$, between the $S = 1/2$ edge spin and the neighboring $S = 1$ spin, and minimized the nonuniformity of the ground state away from the edge.

In the present paper, we start from the usual OBC and modify the amplitude of bond interactions on both ends or place the potential on both edge sites to analyze the boundary condition dependence of the ground state. As for the spin system, the bonds, $J_{\rm edge}$, on both left and right edges are varied. If we place the strong antiferromagnetic bond on one edge, the singlet correlation on that edge is enhanced, and as a result, the correlation on the neighboring bond decreases, which enhances or reduces the inhomogeneity of the ground state. In a similar manner, the electronic states can be tuned by modifying the hopping energy of edge bonds, $t_{\rm edge}$, or by placing the chemical potential on edge sites, $\mu_{\rm edge}$. One can minimize the nonuniformity of the electron density by adjusting the value of $\mu_{\rm edge}$. Furthermore if one uses different values of $\mu_{\rm edge}$ between the two edges, the conduction electrons shift to left or right, and the position of the center of mass of electrons can be controlled.

Besides the system with even number of L, we deal with odd number of L to shift the center of mass of electrons smoothly along the 1D chain in OBC and at the same time keeping electron density constant away from the boundary. Although the average electron filling factor $\rho = N_e/L$ (N_e denotes the electron number) slightly deviates from the one we have in the even-L case, we can pin the excess electrons or holes to the boundary by tuning the value of $\mu_{\rm edge}$.

C. Deformed interactions

Recently, Gendiar, Krcmar, and Nishino proposed an unprecedented analysis to get rid of the boundary effect by deforming the interaction strength of the system following the $\sin^2$ function which decreases from the center toward both ends of the system.[11,18–21]

In this paper we use the following deformed Hamiltonian:

$$\begin{aligned}\mathcal{H} = &\sum_{n=1}^{L-1}\sin^2\left(\frac{\pi n}{L}\right) g(n,n+1)\\ &+\sum_{n=1}^{L-2}\sin^2\left(\frac{\pi(n+1/2)}{L}\right) h(n,n+2)\\ &+\sum_{n=1}^{L}\sin^2\left(\frac{\pi(n-1/2)}{L}\right) u(n),\end{aligned} \tag{8}$$

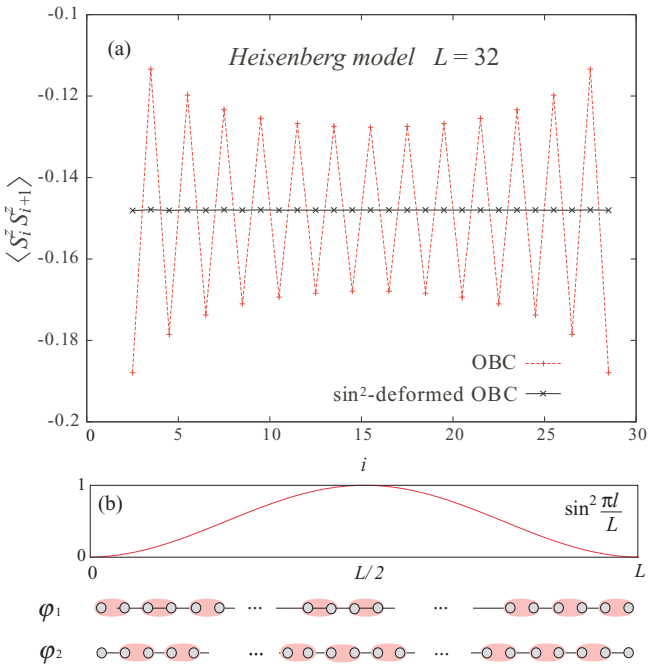

FIG. 1. (Color online) (a) Site dependence of the nearest-neighbor correlation, $\langle S_i^z S_{i+1}^z \rangle$, in the $S = 1/2$ Heisenberg model with OBC and $\sin^2$ deformation at $L = 32$ and $m = 200$. (b) The functional form of the $\sin^2$ deformation in Eq. (8), and the two types of wave function of the dimer state, φ_1 and φ_2, which have the same energy.

where $g(n,n+1)$ is the nearest-neighbor interaction, $h(n,n+2)$ is the next-nearest-neighbor interaction, and $u(n)$ includes the on-site interaction and potential. The uniform chemical potential, μ, is also included as $u(n)$ which is deformed by the prefactor and becomes nonuniform.[19] Figure 1 shows the site dependence of the nearest-neighbor spin-spin correlation of the $S = 1/2$ Heisenberg model, $g(n,n+1) = J\boldsymbol{S}_n \cdot \boldsymbol{S}_{n+1}$, under the usual OBC and under the deformation of interaction. One finds that the usual OBC induces a twofold oscillation which decays slowly toward the system center. The oscillation is fully suppressed by the deformation and the local quantity becomes site independent.

Here, we give an interpretation on these site-independent results. Consider the system with even $L = 2N$. Then, one finds the following relation:

$$\sum_{l=1}^{N} J \sin^2 \frac{\pi(2l)}{L} = \sum_{l=1}^{N} J \sin^2 \frac{\pi(2l-1)}{L}, \tag{9}$$

which means that the sum of the coupling constant is the same between even bonds $(2l)$ and odd bonds $(2l-1)$ [although the total number of even bonds with finite coupling is less than that of odd bonds because $\sin^2(2N\pi/L) = 0$, which corresponds to the missing bond in OBC]. Suppose that we have translational symmetry broken dimer states with twofold periodicity, which are represented by two different types of wave functions, φ_1 and φ_2, as shown in the lower panel of Fig. 1; φ_1 consists of dimers on even bonds and φ_2 consists of those on odd bonds. If either of φ_1 and φ_2 has lower energy than the other, that state is selected as the ground state. However, due to the relation in Eq. (9), φ_1 and φ_2 have the same energy, and thus the translationally symmetric wave function $(\varphi_1 \pm \varphi_2)/\sqrt{2}$ can be constructed, which has the same ground-state energy. Hikihara and Nishino recently calculated the electronic system with this $\sin^2$ deformation and found that the overlap with the PBC wave function is almost 1.[20] This result was in fact supported analytically for the noninteracting case.[21] In the results of the free fermionic model,[11] the Heisenberg chain [Fig. 1(c)], and J_1-J_2 models, which we will see shortly, the translational symmetry is indeed recovered by the deformation. Therefore, we consider that the $\sin^2$ deformation is a condition to have the translationally symmetric ground state at least for simple single-band short-range interacting systems.

III. J_1-J_2 MODEL

A. Dimer order

Our first step is to examine how the order operators discussed in Sec. II A behave under the variation of boundary conditions when the symmetry-breaking long-range order is present in the bulk limit. For this purpose, we choose a J_1-J_2 model, whose Hamiltonian reads

$$\mathcal{H} = \sum_j (J_1 \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1} + J_2 \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+2}), \tag{10}$$

where $J_1 > 0$. The exact ground state at $\alpha = J_2/J_1 = 0.5$, which is called the Majumdar-Ghosh (MG) point, is exactly represented by the product of local dimer states, and thus the dimer-dimer correlation is expected to show no decay for length scale large enough to neglect the boundary effect induced by OBC. The existence of dimer long-range order is established off the MG point in the region of $\alpha \gtrsim 0.24$.[22]

The nearest-neighbor spin-spin correlation operator is given as

$$D_i = \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}, \tag{11}$$

where S_i is the spin operator of site i. We use the dimer operator

$$O_i = D_{i+1} - D_i = \boldsymbol{S}_{i+1} \cdot \boldsymbol{S}_{i+2} - \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} \tag{12}$$

to define the order parameter σ in Eq. (2). When the translational symmetry breaking dimer order is present, the two-point correlation function, $\langle O_i O_j \rangle$, remains finite in the bulk limit.

B. Boundary condition dependence

We now compare the results under three different types of boundary conditions at $J_2/J_1 = 0.4$ where the dimer long-range order is present in the bulk limit. Figure 2 shows the site dependence of the local operator, $\langle S_i^z S_{i+1}^z \rangle = \langle D_i \rangle/3$. Under usual OBC, $\langle D_i \rangle$ shows twofold periodic oscillation with a large amplitude. The amplitude of oscillation is significantly suppressed, when the modified OBC is adopted with $J_{\rm edge} = 0.475J$ on both edge bonds. Further, by the $\sin^2$ deformation, the oscillation is almost completely suppressed and the spatially uniform $\langle S_i^z S_{i+1}^z \rangle$ is obtained, which means that the translational symmetry is recovered. In fact, this deformation gives almost the identical results with that of the PBC given in the same figure. In all cases, the magnitude of $|\langle S_i^z S_{i+1}^z \rangle|$ has only small i dependence. We also plot the results

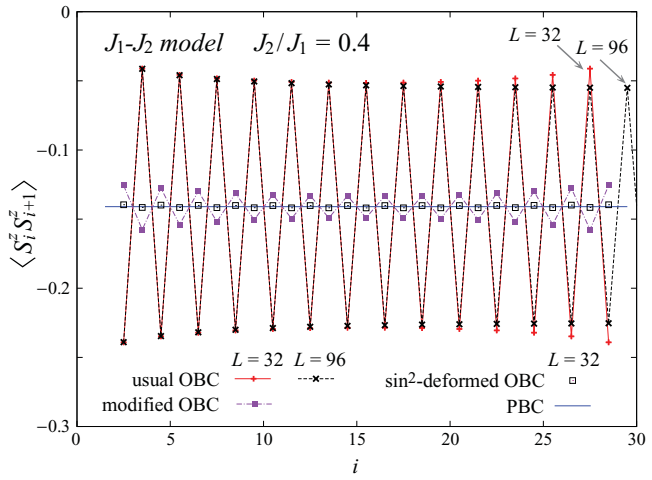

FIG. 2. (Color online) Comparison of local correlation, $\langle S_i^z S_{i+1}^z \rangle$, in the J_1-J_2 model calculated under usual OBC, modified OBC, deformed OBC, and PBC, with $L = 32$ and $m = 200$. The convergence of the results regarding the m dependence is confirmed. For modified OBC we use $J_{\text{edge}} = 0.475J$ on both ends. The results of OBC with $L = 96$ is added to compare with the $L = 32$ one.

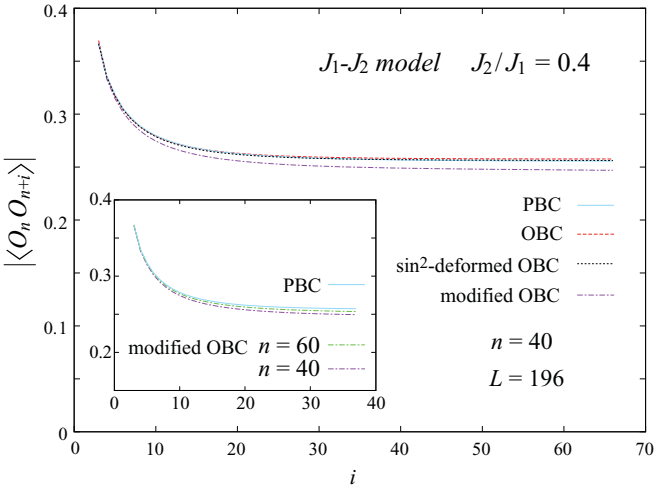

FIG. 3. (Color online) Comparison of two-point correlation functions, $|\langle O_n O_{n+i} \rangle|$, in the J_1-J_2 model with $L = 196$ and $m = 300$. Those of usual OBC, modified OBC, and deformed OBC start from $n = 40$, and the PBC one from $n = 1$. The convergence of the results regarding the m dependence is confirmed. Inset shows the results of modified OBC with $n = 60$ and 40.

under OBC with $L = 96$ to show that the L dependence of the oscillation amplitude is significantly small, indicating that the distinct twofold oscillation remains after the finite-size scaling in OBC. Therefore, there is no doubt that the extrapolated value of $\langle S_i^z S_{i+1}^z \rangle$ in the bulk limit, $\lim_{L\to\infty} \langle D_{L/2} \rangle$, depends severely on the boundary conditions.

Next, we show two-point correlation functions, $|\langle O_n O_{n+i} \rangle|$, in Fig. 3 under the same choices of boundary conditions used in Fig. 2. One finds that all cases almost asymptotically approach a constant value after $i \gtrsim 30$, in sharp contrast to the severely boundary-dependent $\langle D_i \rangle$. The slight difference for the modified boundary condition is due to a boundary effect of finite systems, and it almost vanishes for large $n \gtrsim 60$ as shown in the inset of Fig. 3. From this result, one can safely confirm that the extrapolated value of the two-point correlation function, $\lim_{i\to\infty} |\langle O_n O_{n+i} \rangle|$, is a reliable measure of symmetry-breaking long-range order for any choices of boundary conditions.

IV. KONDO LATTICE MODEL

A. Preliminary information

The next example is devoted to the Kondo lattice model, which is one of the basic models for the heavy-fermionic systems[23] and is studied also as a prototype system to clarify the effects of coupling of localized spins and conduction electrons.[24] The Hamiltonian in one dimension is given as

$$\mathcal{H} = t \sum_j \left(c_{j\sigma}^\dagger c_{j+1\sigma} + \text{H.c.} \right) + J \sum_j \boldsymbol{S}_j \cdot \boldsymbol{s}_j, \qquad (13)$$

where $c_{j\sigma}$ denotes the annihilation operator of the conduction electron at the jth site with spin $\sigma = \uparrow, \downarrow$, and $\boldsymbol{S}_j$ denotes the localized spin operator with $S = 1/2$. $\boldsymbol{s}_j = \frac{1}{2} \boldsymbol{\tau}_{\sigma,\sigma'} c_{j\sigma}^\dagger c_{j\sigma'}$ is the spin operator of the conduction electron with Pauli matrix $\boldsymbol{\tau}_{\sigma,\sigma'}$. The conduction electrons hop with energy t and interact with localized spins through the Kondo exchange coupling J. Its ground state in one dimension is considered as a Tomonaga-Luttinger liquid (TLL) in the weak-coupling region away from half filling. In the strong-coupling region, each conduction electron forms a singlet with localized spins and behaves as a single hole, and the ferromagnetic metallic ground state is realized.[25]

A few years ago, however, there was a proposal by Xavier *et al.* on the possible dimer phase in the region of $J/t \leqslant 1.6$ at quarter filling,[26] which was originally considered a paramagnetic TLL region. Based on the fact that $\langle O_{L/2} \rangle$ calculated under OBC with DMRG seems to remain finite after the size scaling, they claimed that the translational symmetry is broken in the bulk limit. We carried out similar DMRG study on the same model and reproduced their results, but with different conclusions based on the analyses of the boundary effect.[27,28] In fact, the model at $0 \leqslant J/t \leqslant 1$ is in a state which is extremely difficult to analyze even by DMRG established in one dimension.[29]

In the following we show in detail how the two-point correlations as well as the local quantities behave under the variation of boundary conditions, which has distinct differences from those of the dimer phase in the J_1-J_2 model.

B. Modified open boundary

In the KLM the open boundary condition can be modified by the chemical potential $\mu_{\text{edge}} = \mu(1 - \delta)$ and $\mu\delta$ on the left and the right edges, respectively. The value of μ/t is tuned to -1.6 in order to keep the density of charges at quarter filling within the accuracy of 10^{-3} away from the edge sites, and δ is introduced to shift the center of mass of electrons. Figures 4(a) and 4(b) show the site dependencies of the bond kinetic energy $\langle c_i^\dagger c_{i+1} + \text{H.c.} \rangle$ and the nearest-neighbor correlation of localized spins $\langle S_i^z S_{i+1}^z \rangle$ for several choices of δ.

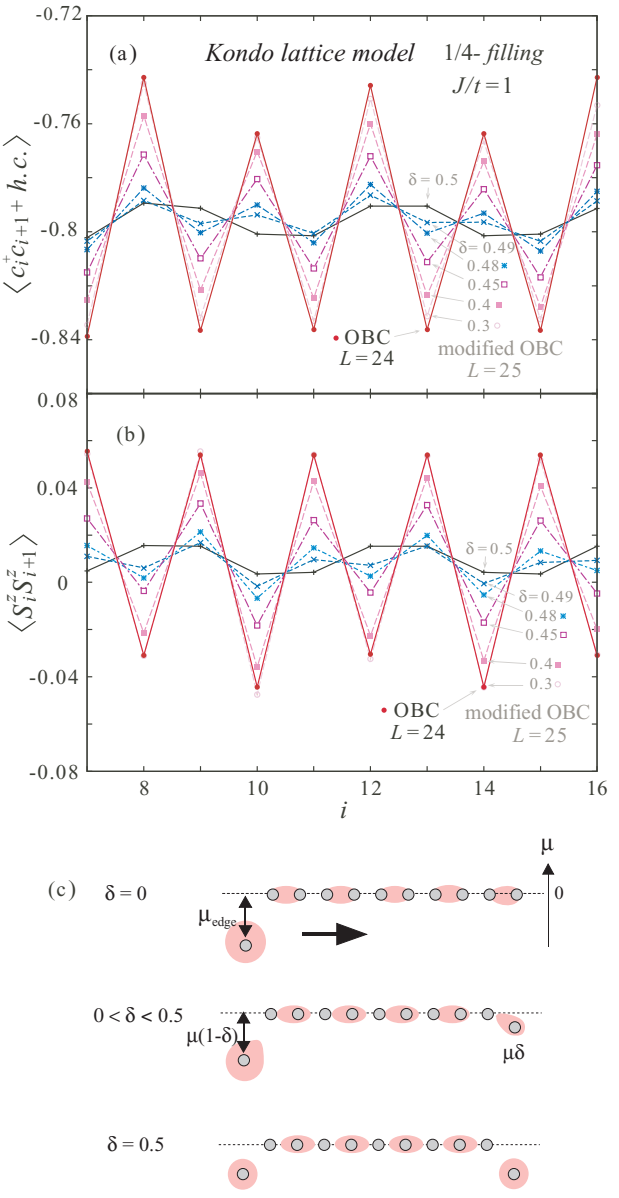

FIG. 4. (Color online) Spatial modulation of two local quantities, (a) bond kinetic energy, $\langle c_i^\dagger c_{i+1} + \text{H.c.}\rangle$, and (b) nearest-neighbor correlation of localized spins, $\langle S_i^z S_{i+1}^z\rangle$, in the Kondo lattice model calculated with usual OBC with $L = 24$ and modified OBC with $L = 25$ with $m = 600$. The convergence of the results regarding the m dependence is confirmed. For modified OBC we use $\mu_{\text{edge}} = \mu(1-\delta)$ and $\mu\delta$ on left and right edge site, respectively, with $\mu/t = -1.6$. (c) Schematic illustration of the electronic states under modified boundary condition by the chemical potential, μ_{edge}. The size of the shaded circles represents the density of conduction electrons.

Under the usual OBC with even L, both $\langle c_i^\dagger c_{i+1} + \text{H.c.}\rangle$ and $\langle S_i^z S_{i+1}^z\rangle$ show large oscillation. The same oscillation is found when the modified boundary is adapted to the odd-L system with $\delta = 0$, namely when μ is placed on only one of the edge sites. From this result, one can understand that μ works to pin the extra charges off quarter filling, $N_e - (L-1)/2$, to the edge site, and the rest of the system remains quarter filled. Then, as δ is increased from 0 toward 0.5, the amplitude of oscillation is gradually suppressed.

Figure 4(c) shows the schematic illustration of the effect of μ and δ on edge sites. The usual OBC with an even number of lattice sites pins the electron density to be the bond-centered spatial modulation along the one-dimensional chain. When the boundary is modified as $0 < \delta < 0.5$, the electrons on the left and right edges have different hopping amplitude to their neighbors, which works to displace the spatial modulation of hoppings and to suppress the oscillation of hopping amplitude as we find in Fig. 4(a). Since the hopping of electrons induces correlations between the local spins through the Kondo exchange interaction, δ also modifies the local spin correlations as shown in Fig. 4(b). This result raises the question of whether the oscillation of $\langle S_i^z S_{i+1}^z\rangle$ found in the OBC is an intrinsic property of the KLM. To study the boundary condition dependence in detail, we next analyze the two-point correlation function of the local spins. Figure 5 shows the dimer-dimer correlation of the local spins $|\langle O_n O_{n+i}\rangle|$. For usual OBC, $|\langle O_n O_{n+i}\rangle|$ saturates toward the finite value already at $i \sim 20$, which apparently suggests the existence of a dimer state. However, when the boundary is modified ($\delta > 0$), the functional form changes significantly and starts to decay monotonously.

To examine whether the odd L of the one-dimensional chain artificially suppresses the dimer correlation or not, we also calculate $|\langle O_n O_{n+i}\rangle|$ of the J_1-J_2 model under both even and odd L starting from $n = 5$ as in KLM, which is shown in the inset of Fig. 5. In the case of the J_1-J_2 model with the true long-range dimer order in the bulk limit, $|\langle O_n O_{n+i}\rangle|$ of the odd L first decays and takes the minimum (or a dip) at around $i \sim 12$ which is near the system center, then shows an upturn, and finally approaches the value of the even L, which is almost an i-independent constant. The local decay (dip) of the dimer correlation is due to the kink structure formed by the phase shift π between the two dimer orders starting from both ends:

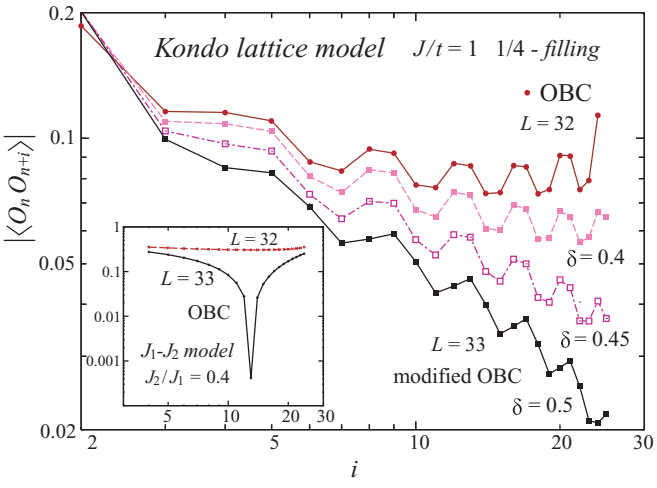

FIG. 5. (Color online) Two-point correlation functions of the dimer operator, $|\langle O_n O_{n+i}\rangle|$ (for fixed $n = 5$) in the Kondo lattice model with $m = 600$ (the m dependence is found to be negligible for the present L's). The usual OBC with $L = 32$ and modified OBC with $L = 33$ for several choices of δ (μ_{edge} is the same as Fig. 4) are compared. The inset shows the two correlation functions, $|\langle O_n O_{n+i}\rangle|$, of the J_1-J_2 model with usual OBC at $L = 32$ and 33 with $n = 5$, to be compared with those of the Kondo lattice model in the main panel.

the misfit of odd L and the twofold periodicity of the dimer order. Since the kink is located around the center of the system, the dimer correlation gradually decreases toward the system center. But for long distances beyond the center of the system, this kink is always located between the two dimer operators O_i and O_j, and the dimer correlation increases up to its original value with an additional phase shift by π.

Such nonmonotonic correlation function is also expected for the KLM of odd L, if the long-range dimer order is present. However, the results in Fig. 5 for finite δ show that the dimer correlation monotonically decreases for long distance even for the case of symmetric edge potentials at $\delta = 0.5$. This result suggests that the dimer order is not an essential property of the KLM at quarter filling at $J = 1$. The large δ dependence of electronic states [see Fig. 4(a)] and concurrently of the spatial structure of localized spins [Fig. 4(b)] are the sign that the electronic state is severely boundary condition dependent, and one should analyze the finite-size scaling and its boundary condition dependence in order to determine the bulk property of the system safely.

C. sin² deformation and periodic boundary

The final set of results is devoted to examining the effect of finite size L and finite number of basis states m in DMRG under the condition where the effect of the missing bond in OBC is as weakened as possible. Based on the discussion in Sec. II C, we perform the calculation under the sin² deformation, which reproduces the translationally invariant wave function for the J_1-J_2 model.

In the KLM, we add uniform chemical potential as n-independent $u(n)$ which is needed to keep the electron density at quarter filling, and deform the Hamiltonian according to Eq. (8). Figure 6(a) shows the comparison of the site dependence of electron density, $\langle n_i \rangle$, between usual OBC and deformed OBC. In usual OBC, the electron density significantly deviates from 0.5 near the system boundary, and as a result, the density around the center slightly exceeds quarter filling. Such deviation due to the boundary effect is

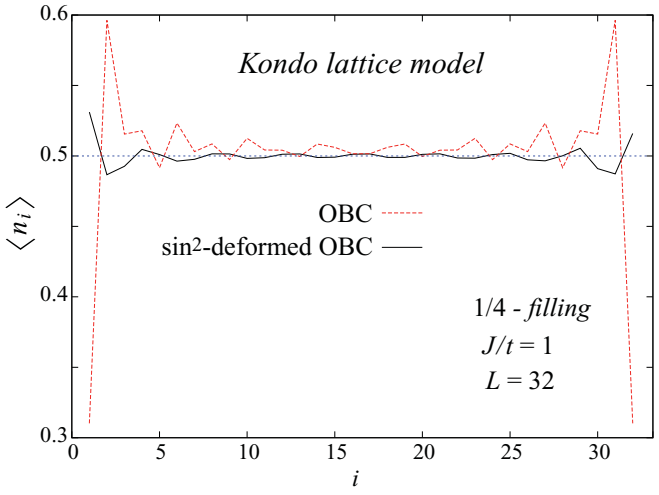

FIG. 6. (Color online) Site dependence of the electron density in the quarter-filled Kondo lattice model at $J/t = 1$, under the usual OBC and sin² deformed OBC with $L = 32$ and $m = 600$.

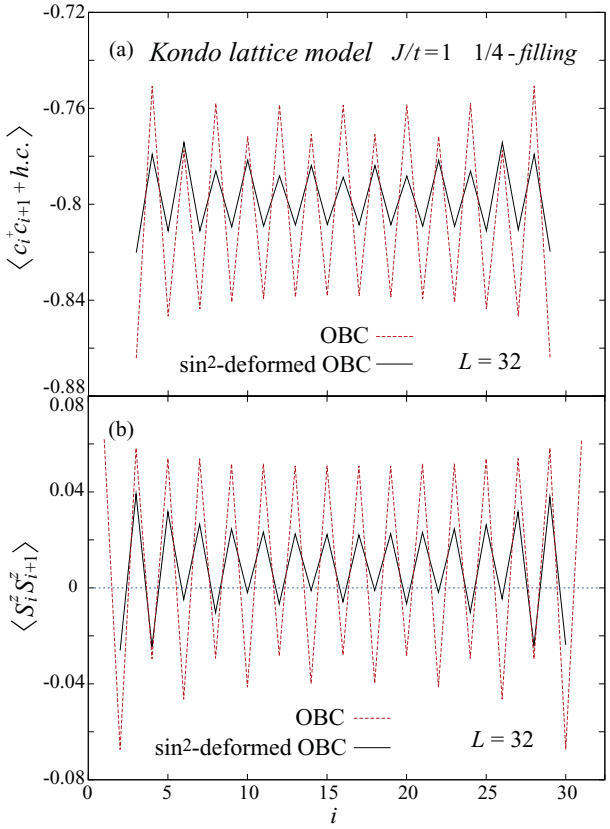

FIG. 7. (Color online) Site dependence of (a) bond kinetic energy, $\langle c_i^\dagger c_{i+1} + \text{H.c.} \rangle$, and (b) nearest-neighbor correlation of localized spins, $\langle S_i^z S_{i+1}^z \rangle$, in the quarter-filled Kondo lattice model at $J/t = 1$, under the usual OBC and sin² deformed OBC with $L = 32$ and $m = 600$.

suppressed in the deformed case, and the electron density becomes nearly site independent. Thus, the results of the latter are guaranteed to be less affected by the missing bond between the two edges.

The comparison of the local quantities of two boundary conditions is given in Fig. 7. The oscillation amplitude of electron hopping, $\langle c_i^\dagger c_{i+1} + \text{H.c.} \rangle$, and the nearest neighbor correlation of localized spins, $\langle S_i^z S_{i+1}^z \rangle$, are both suppressed by the deformation of interaction. It is interesting to find that the mean value of $\langle S_i^z S_{i+1}^z \rangle$ remains a positive finite value even under the deformation. In usual OBC, $\langle S_i^z S_{i+1}^z \rangle$ has a large twofold oscillation between the comparable negative and positive values, and the local spin correlations are characterized by classical $q = \pi/2$ antiferromagnetic state, $\uparrow\uparrow\downarrow\downarrow$. However, by the comparison of the two results, one can conclude that the antiferromagnetic correlation is only stabilized by the boundary effect (the missing bond in usual OBC). The remaining ferromagnetic local correlation seems to be more intrinsic than the antiferromagnetic one in the $J/t = 1$ KLM. In fact, the phase diagram given in Ref. 30 indicates that system at this parameter is very close to the ferromagnetic phase transition.

Finally, we show in Figs. 8(a) and 8(b) the L and m dependencies of the two-point dimer correlation function, $|\langle O_n O_{n+i} \rangle|$. The presented results show the following two important features: The decay of $|\langle O_n O_{n+i} \rangle|$ is always more

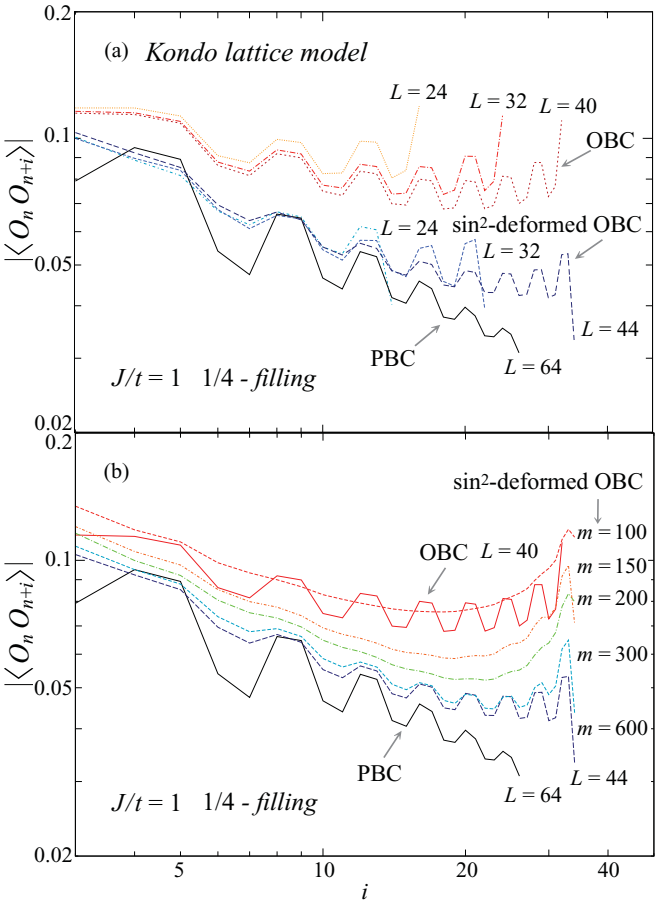

FIG. 8. (Color online) Two-point correlation functions of the dimer operator, $|\langle O_n O_{n+i}\rangle|$ (for fixed $n = 5$) in the Kondo lattice model. (a) Series of results under usual OBC and deformed OBC by varying the system size L. (b) The variation of results of the deformed OBC ($L = 44$) for several choices of m, to be compared with that of the usual OBC with $L = 40$ and $m = 600$. In both panels, the result of PBC with $L = 64$ ($m = 600$ for non-Abelian Hilbert space) is given for comparison.

rapid for larger system size L irrespective of whether we have usual OBC or deformed OBC. Having larger m also leads to the rapid decay in the deformed OBC. Let us discuss the implication of these two features. In general, the accuracy of DMRG is guaranteed by asymptotically restricting the number of bases m needed to reproduce the quantum states. However, this technical advantage may sometimes bring in a by-product when m is not taken large enough: an artificial suppression of intrinsic long-range quantum fluctuation which is required to suppress the boundary-induced symmetry braking. If we focus on the value of $|\langle O_n O_{n+i}\rangle|$ at the particular length i in Fig. 8(a), we always find smaller values for larger L. Since the calculation with larger L includes the component of quantum fluctuation with larger length scale, this fact indicates that the dimer correlation should indeed be suppressed if the system includes a proper long-range quantum fluctuation present in the bulk limit. The same discussion holds for the m dependence: by including a larger number of m, the more the fluctuation effect is included. If such fluctuation is intrinsic, the dimer correlation will be suppressed by the increase of m, which is in fact the case.

Let us briefly comment on the relation of the above L and m scaling with the entanglement entropy. In the systems with small L and m, the number of eigenstates is limited to a small number. This smallness generally enhances the separation of discrete energy levels and suppresses long-range quantum fluctuations, which severely influences the accuracy of long-range two-point correlation functions near the critical point. Meanwhile, the long-range quantum fluctuation generates quantum entanglement between two regions in the system, so that the increase in L and m enhances the entanglement entropy. Therefore, not only the two-point correlation function but also the entanglement entropy shall serve as a measure of to what extent the long-range quantum fluctuation is taken into account near the critical point. The detailed and quantitative analysis on the relation of entanglement entropy with the boundary effect is left as a future problem.

We finally note that the results of these L and m scaling asymptotically approach the one under the PBC in the same panel of Fig. 8. The $|\langle O_n O_{n+i}\rangle|$ of PBC clearly shows an algebraic decay characteristic of the Tomonaga-Luttinger liquid. As discussed in Ref. 11 (see Sec. II), the $\sin^2$ deformation is one of the ways to recover the translational invariance, which is demonstrated in Sec. III for the J_1-J_2 model. To recover perfectly the translational symmetry by the deformation in KLM at $J = 1$ is rather out of scope in the present calculation, because the on-site Kondo singlet correlation competes with the inter-site hopping, and the applicability of the $\sin^2$ deformation is not clear. However, even in such a difficult case, the analysis of the asymptotic behavior of $|\langle O_n O_{n+i}\rangle|$ gives us the strong indication that the true bulk property of the system approaches the one given under PBC, and that the dimer correlation is only induced by the boundary effect. The good coincidence of $|\langle O_n O_{n+i}\rangle|$ in Fig. 5 and Fig. 8 under different series of boundary conditions is regarded as its collateral evidence.

V. SUMMARY AND DISCUSSION

To summarize, we made a case study analysis on the density matrix renormalization group calculation and proposed the systematic treatment to determine whether the symmetry-breaking long-range order exists or not. Since the two-point correlation function in the bulk limit gives the lower bound of the symmetry-breaking long-range order parameter (see Sec. II A), we focused on the two-point correlation functions and systematically studied their boundary condition dependence. We demonstrated the calculations on the two contrasting cases, the J_1-J_2 model which has dimer long-range order, and the Kondo lattice model at quarter filling whose ground state has not reached a consensus yet due to numerical difficulty.

Four different types of boundaries are adopted and their effect on the expectation values of order operators are analyzed. In the usual OBC we always find oscillation of local quantities, e.g., the nearest-neighbor spin-spin correlation $\langle S^z_i S^z_{i+1}\rangle$ or bond kinetic energy $\langle c^\dagger_i c_{i+1} + \text{H.c.}\rangle$ oscillates with the largest amplitude. The modified OBC relaxes the oscillation to some extent under the variation of imbalance between potentials on both edges. Then, the deformation of interactions and PBC basically recover the homogeneity

of local quantities. As the boundary effect fades out in such a way, the two-point correlation function also shows a systematic boundary condition dependence, and thus the degree of inhomogeneity of the local quantities gives a measure of to what extent the boundary effect of OBC is included in the wave function. Therefore, by examining the correspondence of local quantities and the two-point correlation function, one could analyze the overall features of the *boundary effect* as summarized in (III) of Sec. II A.

Such boundary condition dependence is particularly distinct when the system is critical. When the system has symmetry-breaking long-range order (gapped), the two-point correlation function is insensitive to the boundary conditions. This fact is confirmed in the J_1-J_2 model, where the two-point correlation functions reach the same value after the finite-size scaling even when the corresponding local correlations take the significantly different value with each other. By sharp contrast, when the system lacks a distinct gap, the boundary condition severely affects the two-point correlation function as we find in the Kondo lattice model:[28] In OBC it seems to behave convex upward and asymptotically approach a finite value with increasing distance, which is easily transformed to the algebraic decay, once either of the modified OBC, $\sin^2$ deformation, or PBC is adopted. The boundary condition dependence of the two-point correlation function (Figs. 5 and 8) is in good correspondence with that of the local quantities (Figs. 4 and 7), and such boundary-dependent behavior is clearly different from that observed in the J_1-J_2 model. These results show that the dimer correlation observed in OBC is not an intrinsic property of the KLM and that *it is difficult to conclude that the symmetry-breaking long-range order does exist at quarter filling at* $J/t = 1$. This fragile example which requires a difficult numerical treatment provides us with a good lesson that numerical study, although it sometimes becomes as rigorous as analytical techniques, may have much analysis dependence, and one quite often needs care to understand the intrinsic physics lying behind.

We conclude that the DMRG calculation, which is often performed on OBC, sometimes reaches misleading conclusions. While OBC is very useful to analyze the detailed nature of the well-known ground state, we argue that to have a reliable conclusion on the determination of the ground state itself, the examination of the boundary condition dependence on the two-point correlation should be performed.

ACKNOWLEDGMENT

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