# Suppression of finite-size effects in one-dimensional correlated systems

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(Received 7 December 2010; published 19 May 2011)

We investigate the effect of a nonuniform deformation applied to one-dimensional (1D) quantum systems, where the local energy scale is proportional to  $g_j = [\sin(j\pi/N)]^m$  determined by a positive integer m, site index  $1 \le j \le N-1$ , and system size N. This deformation introduces a smooth boundary to systems with open-boundary conditions. When  $m \ge 2$ , the leading 1/N correction to the ground-state energy per bond  $e_0^{(N)}$  vanishes and one is left with a  $1/N^2$  correction, the same as with periodic boundary conditions. In particular, when m = 2, the value of  $e_0^{(N)}$  obtained from the deformed open-boundary system coincides with the uniform system with periodic boundary conditions. We confirm the fact numerically for correlated systems, such as the extended Hubbard model, in addition to 1D free-fermion models.

#### DOI: 10.1103/PhysRevA.83.052118 PACS number(s): 03.65.Aa, 05.30.Fk, 71.10.Fd

## I. INTRODUCTION

Periodic boundary conditions (PBCs) are often more convenient than open-boundary conditions (OBCs), when asymptotic properties of one-dimensional (1D) quantum systems are studied in the thermodynamic limit. This is partially because boundary energy corrections exist under OBCs, where eigenstates are not translationally invariant. Systems with PBCs normally contain smaller finite-size effects, and this property of PBCs is appropriate for accurate determination of bulk properties by means of finite-size scaling [1–3].

In numerical studies of lattice models, OBCs are often chosen for technical reasons. In particular, the majority of practical numerical analyses by the density-matrix renormalization group (DMRG) method [4–6] are performed under OBCs. Concerning finite-size systems with PBCs, the crucial point in DMRG is the ring-shaped geometry, which reduces the decay rate of singular values [7]. Although recent progress in DMRG and tensor product formalisms made it possible to include the PBCs in a natural manner [7–10], numerical implementation requires additional computational resources as compared with conventional DMRG analyses.

A way of suppressing the boundary energy corrections induced by OBCs is to introduce smooth boundary conditions (SBCs) [11,12]. Recently we proposed a variant of the SBCs, where the local energy scale of N-site systems is proportional to the deformation function  $[\sin(j\pi/N)]^2$  specified by the site index  $1 \le j \le N-1$  [13,14]. This sine-squared deformation (SSD) [15] completely suppresses the boundary effects when the ground-state energy of a free-fermion model on a 1D lattice is considered. In this paper we generalize the deformation function, which is given by  $g_j = [\sin(j\pi/N)]^m$ , where m is a positive integer [16]. In the next section, we examine the effect of this sinusoidal deformation by  $g_j$  up to m=5 when it is applied to the 1D free-fermion model. It is shown that the case m=2, the SSD, is the most efficient for the suppression of the boundary effect.

Another trial in this paper is the application of SSD to correlated systems. As typical examples of correlated systems,

we choose the spinless-fermion model with nearest-neighbor interaction and the extended Hubbard model; we report the numerical result obtained by DMRG in Sec. III. When the interaction is present, the determination of the chemical potential is nontrivial. We present a systematic way of solving this problem in Sec. IV. We summarize results in the last section.

# II. SINUSOIDAL DEFORMATION

We start from the sinusoidal deformation applied to the free-fermion model on the 1D lattice. Consider a tight-binding model represented by the Hamiltonian

$$\mathcal{H}^{(N)} = -t \sum_{i=1}^{N-1} (c_j^{\dagger} c_{j+1} + c_{j+1}^{\dagger} c_j) - \alpha t (c_N^{\dagger} c_1 + c_1^{\dagger} c_N), \quad (1)$$

where N is the system size, and t is the hopping energy. Operators  $c_j^{\dagger}$  and  $c_j$  represent the creation and annihilation of fermions, respectively. The parameter  $\alpha$  specifies the boundary condition, where OBCs and PBCs correspond to  $\alpha=0$  and  $\alpha=1$ , respectively. (The choice  $\alpha=-1$  is known as the antiperiodic boundary conditions, which we do not treat in this paper.) For each boundary condition, the one-particle energy is expressed as

$$\varepsilon_{\ell} = \begin{cases} -2t \cos\left(\frac{\pi \ell}{N+1}\right) & \text{for OBC} \quad (\alpha = 0), \\ -2t \cos\left(\frac{2\pi \ell}{N}\right) & \text{for PBC} \quad (\alpha = 1), \end{cases}$$
 (2)

where the energy index  $\ell$  runs from 1 to N. The ground-state energy  $E_0^{(N)}$  at half filling is obtained as the sum of  $\varepsilon_\ell$  below the Fermi energy  $\varepsilon_{\rm F}=0$ .

Throughout this paper we focus on the system size dependence on the energy per site  $E_0^{(N)}/N$  or the energy per bond, which is  $E_0^{(N)}/N$  under PBCs and is  $E_0^{(N)}/(N-1)$  under OBCs. After a short algebra, one obtains

$$\frac{E_0^{(N)}}{N} = -\frac{2t}{\pi} + \frac{t}{N} \left( 1 - \frac{2}{\pi} \right) + O\left(\frac{1}{N^2}\right) \tag{3}$$

with OBCs, where the leading order of the finite-size correction is proportional to  $N^{-1}$ . The correction of the same order also exists for the energy per bond. With PBCs, one finds

$$\frac{E_0^{(N)}}{N} = -\frac{2t}{\pi} + \frac{2\pi t}{3N^2} + O\left(\frac{1}{N^3}\right),\tag{4}$$

where the leading correction is of the order of  $N^{-2}$ . The difference between Eqs. (3) and (4) chiefly comes from the presence of the boundary energy which exists only when OBCs are imposed.

The sinusoidal deformation introduces a positiondependent energy scale  $g_j = [\sin(j\pi/N)]^m$  to each bond of the system with OBCs, where m is the positive integer [13,14]. Deforming  $\mathcal{H}^{(N)}$  in Eq. (1), we obtain the corresponding free-fermionic Hamiltonian

$$\mathcal{H}_{\text{sine}}^{(N)} = -t \sum_{j=1}^{N-1} \left[ \sin \left( \frac{j\pi}{N} \right) \right]^m (c_j^{\dagger} c_{j+1} + c_{j+1}^{\dagger} c_j).$$
 (5)

We have not obtained an analytical solution for the one-particle spectrum of  $\mathcal{H}_{\text{sine}}^{(N)}$  so far, except for the zero-energy state. Thus we perform numerical analyses in the following investigations on the ground state.

Since we are interested in the ground-state energy per site (or per bond), we introduce the normalization factor

$$B^{(N)} = \sum_{j=1}^{N-1} \left[ \sin \left( \frac{j\pi}{N} \right) \right]^m = \sum_{j=1}^{N-1} g_j, \tag{6}$$

which is the sum of the deformation factors over the entire system. When m is an odd positive integer, we have

$$B^{(N)} = \sum_{\ell=0}^{(m-1)/2} \frac{(-1)^{\ell}}{(2\ell)^{m-1}} \binom{m}{\ell} \cot \left[ \frac{(m-2\ell)\pi}{2N} \right], \quad (7)$$

and when m is an even positive integer, we have

$$B^{(N)} = \frac{N}{2^m} \begin{pmatrix} m \\ m/2 \end{pmatrix}. \tag{8}$$

We represent the ground-state energy of  $\mathcal{H}_{\text{sine}}^{(N)}$  at half filling by the notation  $E_0^{(N)}$ . It is expected that the normalized energy

$$e_0^{(N)} = \frac{E_0^{(N)}}{B^{(N)}} \tag{9}$$

converges to  $-2t/\pi$  in the large N limit in analogy to Eqs. (3) and (4). We refer to  $e_0^{(N)}$  in Eq. (9) as the energy per bond in the following. As a convention, we set  $B^{(N)} = N - 1$  for the system with OBCs, and  $B^{(N)} = N$  with PBCs, where these values just represent the number of bonds. Using this extended definition of  $B^{(N)}$ , we can represent the energy per bond by Eq. (9) regardless of the boundary condition or the presence of deformation.

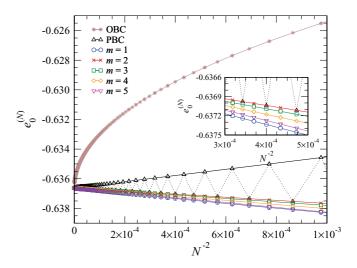


FIG. 1. (Color online) Convergence of  $e_0^{(N)}$  in Eq. (9) with respect to N at half filling. We choose t as the unit of the energy. Data with OBCs, PBCs, and the deformed cases with m=1-5 are shown.

We regard t as the unit of the energy in the numerical analyses. Figure 1 shows the N dependence of  $e_0^{(N)}$  in Eq. (9) for the undeformed systems with OBCs, PBCs, and the deformed systems from m=1 to 5. When the PBCs are imposed, the convergence of  $e_0^{(N)}$  with respect to  $N^{-2}$  is linear, and there is an even-odd oscillation with respect to the particle number N/2. Similarly, the linear  $N^{-2}$  dependence is observed when  $m \ge 2$  under the sinusoidal deformation. In the case m=1, there is an additional logarithmic correction, as will be shown later. It should be noted that when the particle number N/2 is odd,  $e_0^{(N)}$  obtained with the sinusoidal deformation for m=2 coincides with  $e_0^{(N)}$  obtained with PBCs [17]. This complete agreement is checked down to the smallest digit in numerical precision. Throughout this paper we use the exact diagonalization in order to reduce any numerical errors to minimum.

In order to confirm the  $N^{-2}$  dependence of  $e_0^{(N)}$  with the sinusoidal deformation under  $m \ge 2$ , we plot the difference between  $e_0^{(N)}$  obtained with PBCs (when N/2 is even) and  $e_0^{(N)}$  with the sinusoidal deformation. To avoid any confusion, let  $E_{\rm PBC}^{(N)}$  and  $E_{\rm sine}^{(N)}$  denote the ground-state energy obtained with PBCs and with the sinusoidal deformation, respectively. We also use similar notation for the normalization factors  $B_{\rm PBC}^{(N)} = N$  and  $B_{\rm sine}^{(N)}$  for the normalization factor defined in Eq. (6). Figure 2 depicts the magnified difference

$$N^{2} \left[ e_{\text{PBC}}^{(N)} - e_{\text{sine}}^{(N)} \right] \equiv N^{2} \left[ \frac{E_{\text{PBC}}^{(N)}}{B_{\text{PBC}}^{(N)}} - \frac{E_{\text{sine}}^{(N)}}{B_{\text{sine}}^{(N)}} \right]$$
(10)

when N is even. It is shown that the logarithmic correction  $N^{-2} \log N$  is present when m = 1, and is absent when  $m \ge 2$ .

Figure 3 shows the spatial distribution of the bond correlation function  $\langle c_j^{\dagger} c_{j+1} + c_{j+1}^{\dagger} c_j \rangle$  at half filling when N=1000. The Friedel oscillations induced by the boundary are clearly observed when OBCs are imposed (the asterisks), and weaker oscillations are observed with the sinusoidal deformation when m=1. Only when m=2, there are no oscillations at all; we

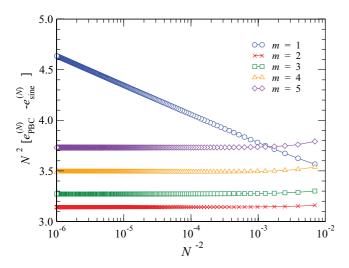


FIG. 2. (Color online) Asymptotic behavior of  $e_0^{(N)}$  for the deformed chains when  $1 \le m \le 5$  with respect to  $e_0^{(N)}$  of the system with PBCs. We choose t as the unit of the energy. A logarithmic correction is present when m = 1.

checked the uniformity (the translation invariance) of the bond correlation function down to 16 digits in numerical precision. When  $m \ge 3$ , the boundary effects appear again. In this case the bond correlation function toward the system boundary does not oscillate, and decreases in monotonic manner. Such behaviors for each m might be related to the suppression of the boundary corrections in  $e_0^{(N)}$ .

We compare the efficiency of SSD (m=2) with the SBCs proposed in Refs. [11] and [12]. Figure 4 shows the bond correlation function for both cases at half filling, where the length of the boundary area in the SBC is chosen as M=10 and 30 when the system size is N=1000. Although bulk property is well captured by the SBC already for M=30, boundary fluctuations are still present. On the other hand, the bond correlation function is almost uniform away of the boundary.

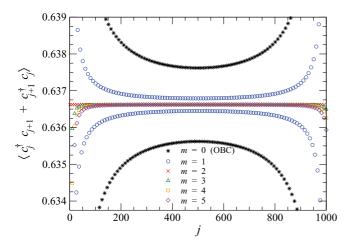


FIG. 3. (Color online) Expectation value of the bond correlation function  $\langle c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j \rangle$  with respect to j under sinusoidal deformation.

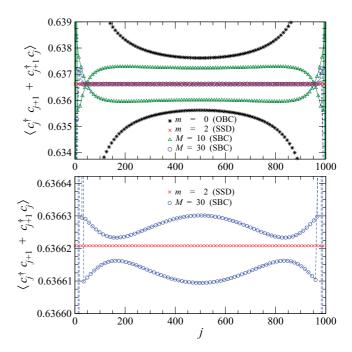


FIG. 4. (Color online) Comparison of the expectation value of the bond correlation function at half filling under SSD (m = 2) and a SBC in Refs. [11] and [12]. The number M in the case of the SBC specifies the length of area where the interactions are modified near the system boundary. The bottom graph shows the numerical details when M = 30 (SBC) with respect to SSD.

Now we discuss the way of treating the deformed system away from half filling. For the undeformed systems with OBCs or PBCs, it is sufficient to include the chemical potential term  $-\mu \sum_{j=1}^{N} n_j$  in Eq. (1), where  $n_j = c_j^{\dagger} c_j$  is the number operator. The value of  $\mu$  adjusts the Fermi energy to zero, and is given by

$$\mu(f) = -2t\cos(\pi f),\tag{11}$$

where f is the filling factor,

$$f = \frac{1}{N} \sum_{j=1}^{N} \langle n_j \rangle. \tag{12}$$

A natural way of introducing  $\mu(f)$  under the sinusoidal deformation is to write down the Hamiltonian as a sum of the local terms,

$$\mathcal{H}_{\text{sine}}^{(N)} = \sum_{j=1}^{N-1} \left[ \sin \left( \frac{j\pi}{N} \right) \right]^m h_{j,j+1} = \sum_{j=1}^{N-1} g_j h_{j,j+1}, \quad (13)$$

where  $\mu(f)$  is included in the bond operator,

$$h_{j,j+1} = -t(c_j^{\dagger}c_{j+1} + c_{j+1}^{\dagger}c_j) - \frac{\mu}{2}(n_j + n_{j+1}). \tag{14}$$

In order to confirm the validity of these constructions in Eqs. (11)–(14), we carried out numerical calculations for the selected fillings f=1/4 and f=1/8. Figure 5 shows the  $N^{-2}$  dependence of  $e_0^{(N)}=E_0^{(N)}/B^{(N)}$ , where  $E_0^{(N)}$  is the ground-state energy for each filling. We plot the data only when the particle number  $p\equiv fN$  is even. Analogous to half filling, the bond energy  $e_0^{(N)}$  with PBCs coincides with that obtained

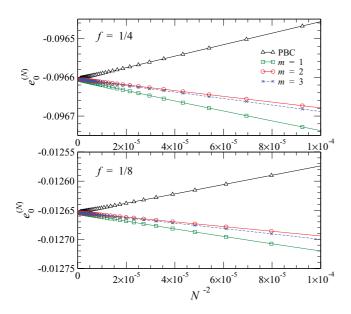


FIG. 5. (Color online) Convergence of  $e_0^{(N)}$  with respect to  $N^{-2}$  at 1/4 filling and 1/8 filling. We choose t as the unit of the energy.

with a SSD (m = 2) when p is odd [17]. The logarithmic corrections are again present when m = 1.

The uniformity of the ground state obtained with the sinusoidal deformation is checked by calculating the occupancy  $\langle n_j \rangle = \langle c_j^\dagger c_j \rangle$  at f = 1/2, 1/4, and 1/8. Figure 6 shows  $\langle n_j \rangle$  when m = 1, 2, and 3. At half filling,  $f = 1/2, \langle n_j \rangle$  is always equal to 1/2 by the particle-hole symmetry. Even away from the half filling, this uniformity is kept when m = 2. There are

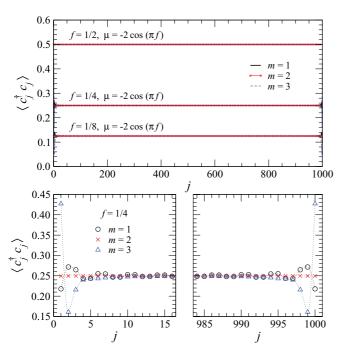


FIG. 6. (Color online) Position dependence of the occupation number  $\langle n_j \rangle = \langle c_j^\dagger c_j \rangle$  at f=1/2,1/4, and 1/8 when m=1,2, and 3 (upper graph). The left-hand and right-hand lower graphs display the occupancy at f=1/4 close to the boundaries.

small fluctuations near the system boundary when m = 1 and 3. In this way, the construction of Hamiltonian in Eqs. (13) and (14) away from half filling is justified, especially for the SSD.

#### III. CORRELATED SYSTEMS

It is expected that the SSD reduces the boundary effect even when interactions are present between particles. In order to check this conjecture, we apply the sinusoidal deformation to correlated systems by means of the Hamiltonian Eq. (13) written in the linear combination of bond operators. We study the system size dependence of the ground-state energy  $E_0^{(N)}$  and the uniformity of the system.

## A. Spinless fermions

As an example, let us consider spinless fermions on the 1D lattice, whose behavior is described by the uniform Hamiltonian,

$$\mathcal{H}_{PBC}^{(N)} = -t \sum_{j=1}^{N} (c_{j}^{\dagger} c_{j+1} + c_{j+1}^{\dagger} c_{j}) + V \sum_{j=1}^{N} \left( c_{j}^{\dagger} c_{j} - \frac{1}{2} \right) \left( c_{j+1}^{\dagger} c_{j+1} - \frac{1}{2} \right)$$
(15)

with PBCs, where the system contains the repulsive Coulomb interaction V>0 between neighboring sites, in addition to the hopping amplitude t. In this section we restrict ourselves to the half-filled case only, therefore the chemical potential  $\mu$  is zero [18]. The construction of the Hamiltonian with OBCs and its sinusoidal deformation is analogous to what we have done in the previous section. The deformed Hamiltonian can be defined by putting the bond operator as

$$h_{j,j+1} = -t(c_j^{\dagger} c_{j+1} + c_{j+1}^{\dagger} c_j) + V(c_j^{\dagger} c_j - \frac{1}{2})(c_{j+1}^{\dagger} c_{j+1} - \frac{1}{2})$$
(16)

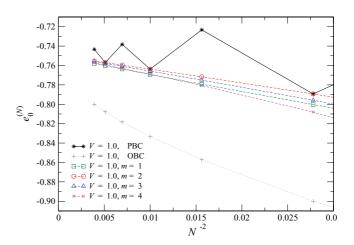


FIG. 7. (Color online) Energy per bond  $e_0^{(N)}$  of the spinless fermion model at V=1 up to N=16. We choose t as the unit of the energy.

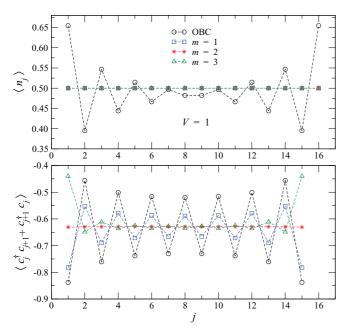


FIG. 8. (Color online) Occupation number  $\langle n_j \rangle$  and the bond correlation  $\langle c_i^{\dagger} c_{j+1} + c_{j+1}^{\dagger} c_j \rangle$  when V = 1 at half filling.

and substituting it into Eq. (14). We calculate the ground state

and the corresponding energy  $E_0^{(N)}$  at half filling up to N=16. Figure 7 shows  $e_0^{(N)}$  with respect to  $N^{-2}$ . When the sinusoidal deformation is applied, we observe the same  $N^{-2}$  dependence as was seen for the noninteracting case. In particular, when N/2 is odd,  $e_0^{(N)}$  obtained for m=2 shows good agreement with the result from the PBC. The coincidence, however, becomes less accurate with increasing V, and there is a deviation  $\sim 0.2\%$  in  $e_0^{(N)}$  when V=5. Figure 8 shows the occupation number  $\langle n_j \rangle$  and the bond correlation  $\langle c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j \rangle$  when V=1 at half filling. A clear uniformity is observed when m=2 as shown in the noninteracting cases.

#### **B.** Extended Hubbard model

Now we consider the extended Hubbard model, which contains the on-site Coulomb interaction U and the neighboring interaction V. In this case there is a spin degree of freedom  $(\sigma = \uparrow, \downarrow)$ , and therefore creation and annihilation operators, respectively, are represented as  $c_{j\sigma}^{\dagger}$  and  $c_{j\sigma}$  . The bond operator of the extended Hubbard model is represented as

$$h_{j,j+1} = -t \sum_{\sigma=\uparrow,\downarrow} (c_{j\sigma}^{\dagger} c_{j+1\sigma} + c_{j+1\sigma}^{\dagger} c_{j\sigma})$$

$$+ \frac{U}{2} \left[ \left( n_{j\uparrow} - \frac{1}{2} \right) \left( n_{j\downarrow} - \frac{1}{2} \right) + \left( n_{j+1\uparrow} - \frac{1}{2} \right) \left( n_{j+1\downarrow} - \frac{1}{2} \right) \right]$$

$$+ V(n_{j\uparrow} + n_{j\downarrow} - 1)(n_{j+1\uparrow} + n_{j+1\downarrow} - 1). \quad (17)$$

To avoid the complexity of determining the chemical potential  $\mu$ , we consider the half-filled case where  $\mu = 0$  is guaranteed by the particle-hole symmetry. Figure 9 shows the  $N^{-2}$ 

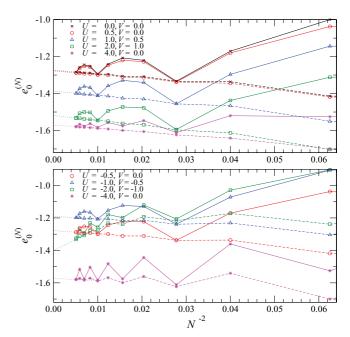


FIG. 9. (Color online) System size dependence of  $e_0^{(N)}$  of the extended Hubbard model at half filling. We choose t as the unit of the energy. The full and the dashed lines connect the energies  $e_0^{(N)}$ obtained by the PBC and SSD, respectively.

dependence of  $e_0^{(N)}$  for various combinations of U and V. The coincidence between the PBC and SSD at half filling occurs when the total number of both up- and down-spin fermions are odd.

The occupancy  $\langle n_j \rangle = \langle n_{j\uparrow} + n_{j\downarrow} \rangle$  and the bond correlation function  $\sum_{\sigma} \langle c_{j\sigma}^{\dagger} c_{j+1\sigma} + c_{j\sigma}^{\dagger} c_{j+1\sigma} \rangle$  at half filling are shown in Fig. 10. The occupancy  $\langle n_j \rangle$  with OBC is clearly

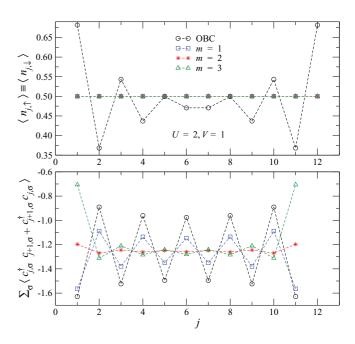


FIG. 10. (Color online) Occupation  $\langle n_{j\uparrow} \rangle = \langle n_{j\downarrow} \rangle$  and the bond correlation  $\sum_{\sigma} \langle c_{j\sigma}^{\dagger} c_{j+1} + c_{j+1\sigma}^{\dagger} c_{j\sigma} \rangle$  of the extended Hubbard model at half filling.

influenced by the system boundaries, whereas the sinusoidal deformations  $(m \ge 1)$  lead to almost constant distribution. The case with m = 2 (asterisks) realizes the minimal position dependence. The bond correlation function is influenced by the boundaries in all cases, and the position dependence is the weakest when m = 2.

#### IV. CHEMICAL POTENTIAL

So far we have not discussed the proper value of the chemical potential  $\mu$  away from the half filling when the interaction is present. The chemical potential term  $-\frac{\mu}{2}(n_{j\uparrow}+n_{j\downarrow}+n_{j+1\uparrow}+n_{j+1\downarrow})$  has to be included to the bond operator in Eq. (18). In the Hartree-Fock or the Fermi-liquid picture,  $\mu$  is adjusted so that the particle number  $p=\sum_{j=1}^N \langle n_{j\uparrow}+n_{j\downarrow}\rangle$  coincides with the number of negative-energy quasiparticle states. The number of particles is independently represented by the derivative of  $E_0^{(N)}$  with respect to  $\mu$ . Thus, the relation  $p=-\partial E_0^{(N)}/\partial \mu$  must be satisfied for the targeted particle number p. Within the sinusoidal deformation, this relation is slightly modified as

$$p = -\frac{N}{B^{(N)}} \frac{\partial E_0^{(N)}}{\partial \mu} = -\frac{\partial N e_0^{(N)}}{\partial \mu},\tag{18}$$

according to the position dependence in the energy scale.

We plot the absolute value  $|p - (-\partial N e_0^{(N)}/\partial \mu)|$  with respect to  $\mu$  for the extended Hubbard model in Fig. 11, under the SSD. The numerical analysis by exact diagonalization gives  $\mu = -4.1425$  for the case N = 12, p = 4, U = 2, and V = 1. Figure 12 shows the corresponding occupation and the bond correlation functions. There is a slight position dependence, since we are dealing with a relatively small system size with a few particles. The position dependence

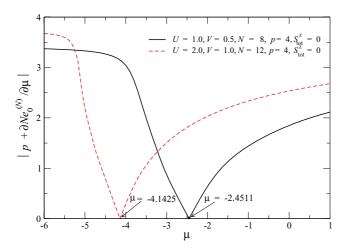


FIG. 11. (Color online) The  $\mu$  dependence of  $|p + \partial N e_0^{(N)}/\partial \mu|$  for the two cases  $f \equiv p/2N = 1/4$  and 1/6. We choose t and  $\mu$  as the units of the energy.

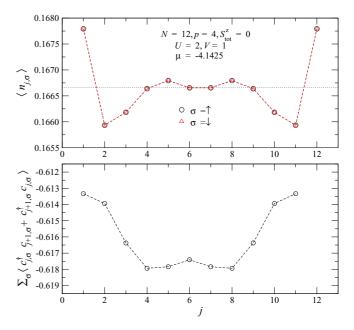


FIG. 12. (Color online) The upper and lower graphs show the occupancy  $\langle n_{i,\sigma} \rangle$  and the bond correlation  $\sum_{\sigma} \langle c_{j\sigma}^{\dagger} c_{j+1\sigma} + c_{j+1\sigma}^{\dagger} c_{j\sigma} \rangle$  at f = 1/6.

becomes conspicuous if we choose either an inaccurate value of  $\mu$  or we consider the deformations with  $m \neq 2$ .

# V. CONCLUSION AND DISCUSSION

We have shown that the sine-squared deformation is the optimal choice if applied to 1D quantum Hamiltonians and it improves convergence of the ground-state energy per bond (or per site)  $e_0^{(N)}$  toward the thermodynamic limit if compared to the uniform systems with open-boundary conditions. Such suppression of the boundary effects is confirmed also for interacting systems, typically for the extended Hubbard model.

We have not determined the "canonical" form of the sinusoidal deformation in the case where there are long-range interactions. It is reported that a small but finite residual boundary effect appears in spin chains which includes the next-nearest-neighbor interaction [15]. Application of the sinusoidal deformation to higher-dimensional quantum systems could be a future problem.

A theoretical puzzle of the sinusoidal deformation remains in coincidence of the ground-state energy calculated with the PBC and SSD. The agreement is almost perfect, which strongly suggests a hidden algebraic relation between these two cases.

### ACKNOWLEDGMENTS

We thank T. Hikihara, A. Feiguin, and K. Okunishi for valuable discussions. This work was supported by ERDF OP R&D, Project "QUTE–Centre of Excellence for Quantum Technologies" (ITMS 26240120009), CE QUTE SAV, APVV-51-003505, VVCE-0058-07, and VEGA-2/0633/09. T.N. acknowledges the support of Grant-in-Aid for Scientific Research (C) No. 22540388.

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