Tomonaga-Luttinger-liquid criticality: Numerical entanglement entropy approach

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The von Neumann entanglement entropy is studied with the density-matrix renormalization-group technique. We propose a simple approach to calculate the central charge using the entanglement entropy for a one-dimensional (1D) quantum system. This approach is applied to a couple of quantum systems: (i) a 1D frustrated spin model and (ii) a 1D half-filled spinless fermions with nearest-neighbor repulsion; it is confirmed that the central charge is estimated very accurately for the both systems. Also, a new method to determine the critical point between Tomonaga-Luttinger-liquid and gapped (or ordered) phases from the proposed approach is suggested. Furthermore, we mention that the Tomonaga-Luttinger parameter can be obtained in a like manner as the central charge, using the charge-density fluctuation of a part of the 1D system.

I. INTRODUCTION

Quantum entanglement[1] is a quantum-mechanical phenomenon created by the separation of interacting quantum particles. This fundamental concept underpins a wide range of research in physics, such as quantum information, quantum computing, and quantum gravity. When one considers this phenomenon in a study, it is often quantified as an *entanglement entropy*. In the field of condensed-matter physics, the von Neumann entanglement entropy has been frequently used as an order parameter to investigate quantum phase transition or topological order in the quantum many-body problems. In particular, for one-dimensional (1D) quantum systems the entropy can be directly related to the *central charge* of the conformal field theory (CFT).[2,3] To date, a method with this relation has been developed as a powerful tool to study the universal properties of the Tomonaga-Luttinger (TL) liquid,[4] combined with numerical methods such as exact diagonalization (ED) or density-matrix renormalization-group (DMRG)[5] techniques.

Let us consider a quantum 1D periodic system with length L. The von Neumann entanglement entropy of its subsystem with length l is given as $S_L(l) = -\text{Tr}_l \rho_l \log \rho_l$, where $\rho_l = \text{Tr}_{L-l} \rho$ is the reduced density matrix of the subsystem and ρ is the full density matrix of the whole system. Using the CFT, the entropy of the subsystem with length l for a fixed system length L has been derived:[2,3,6]

$$S_L(l) = \frac{c}{3} \ln \left[\frac{L}{\pi} \sin \left(\frac{\pi l}{L} \right) \right] + s_1, \tag{1}$$

where c is the central charge of the associated CFT and s_1 is a nonuniversal constant. A prime objective of using this formula is to estimate the central charge,[7–9] which provides definitive information concerning the universality class of a $(1+1)$-dimensional system.[10] This estimation has been applied to a variety of fermionic systems, e.g., with impurity,[11–13] coupled to bosons,[14,15] and under the magnetic field.[16] Although the central charge can be also obtained by examining the finite-size correction of ground-state energy or the low-temperature behavior of specific heat,[17] excited states have to be taken into account and considerable difficulty is involved in the ED and DMRG calculations. But, if one uses Eq. (1), it is only necessary to consider the ground state.

So far, two kinds of numerical methods have been principally adopted to extract the value of c from Eq. (1): one is direct fitting of $S_L(l)$ as a function of l for a fixed system length and the other is scaling analysis using a relation $\Delta S \equiv S_L(\frac{L}{2}) - S_{L'}(\frac{L'}{2}) \simeq \frac{c}{3} \ln \frac{L}{L'}$, considering two systems with lengths L and L'. However, one would encounter difficulty attributable to a finite-size effect in their practical use. More specifically, in the former method Eq. (1) is exact only in the thermodynamic limit $L \to \infty$ and some ambiguity remains in the fitting of the finite-size result,[18] whereas in the latter method the system length to be studied must be strongly restricted due to the incommensurability (or frustration) of spin and/or charge fluctuations as well as the (open-) shell problem in itinerant systems. Therefore, the aim of this paper is to propose a method that overcomes those problems. We first derive an efficient formula for calculating the central charge. And then, to ascertain the validity of the formula, we apply it to a couple of 1D quantum systems: (i) a frustrated spin model and (ii) an itinerant model with strong charge fluctuation. We demonstrate that a very accurate estimation of the critical point between TL-liquid and gapped (or ordered) states is enabled with this method. Furthermore, we suggest that the TL parameter can be calculated in a like manner as the central charge.

II. DERIVATION OF THE FORMULA

Let us now derive the formula for estimating the central charge. We first prepare $S_L(\frac{L}{2})$ and $S(\frac{L}{2} - 1)$ from Eq. (1). Then, by subtracting the one from the other, a simple expression is obtained:

$$c = \frac{3 \left[S_L \left(\frac{L}{2} - 1 \right) - S_L \left(\frac{L}{2} \right) \right]}{\ln \left[\cos \left(\frac{\pi}{L} \right) \right]} \equiv c_1. \tag{2}$$

Using this expression we can easily calculate the central charge for a 1D system with a fixed system length. The main advantages of Eq. (2) are: (i) the nonuniversal constant s_1 does not appear explicitly; (ii) only two values of $S_L(l)$ at the middle of the system, where the finite-size correction to Eq. (1) is the smallest[18] and the DMRG calculation is the most accurate, are used; and (iii) a unique value of c is estimated for each system length and it enables us to perform a systematic extrapolation to the thermodynamic limit. Also, an alternative

expression can be derived from the second derivative of Eq. (1) with respect to l. Since $S_L(l)$ is symmetric about $l = \frac{L}{2}$, i.e., $S_L(l) = S_L(L - l)$, we obtain

$$
\begin{aligned}
c &= -\frac{3L^2}{\pi^2} \left. \frac{\partial^2 S_L(l)}{\partial l^2} \right|_{l=\frac{L}{2}} \\
&\simeq \frac{6L^2}{\pi^2} \left[S_L\left(\frac{L}{2}\right) - S_L\left(\frac{L}{2} - 1\right) \right] \equiv c_2.
\end{aligned}
\tag{3}
$$

Note that Eq. (3) can be also derived by applying $\ln[\cos(\frac{\pi}{L})] \simeq -\frac{\pi^2}{2L^2}$ into Eq. (2).

III. APPLICATION TO QUANTUM SYSTEMS

A. Frustrated spin chain

In order to confirm the validity of Eqs. (2) and (3), we apply them to a couple of 1D quantum systems. The first system considered is the $S = \frac{1}{2}$ frustrated Heisenberg chain. The Hamiltonian is given by

$$
H = J_1 \sum_i \vec{S}_i \cdot \vec{S}_{i+1} + J_2 \sum_i \vec{S}_i \cdot \vec{S}_{i+2},
\tag{4}
$$

where $\vec{S}_i$ is a half-spin operator at site i. The parameters J_1 and J_2 are nearest-neighbor and next-nearest-neighbor antiferromagnetic exchange interactions, respectively. This system has been extensively studied both analytically and numerically:[19–24] the ground state is of a dimerized zig-zag-bond state for $0.241 \lesssim J_2/J_1 \leqslant 0.5$ and of the Majumdar-Ghosh state with incommensurate spiral correlations for $J_2/J_1 \geqslant 0.5$; accordingly, the spin gap opens when $J_2/J_1 \gtrsim 0.241$. For $J_2/J_1 \lesssim 0.241$ the system is described as a TL liquid and the central charge is expected to be unity ($c = 1$). In recent years this system has been frequently used as a touchstone of numerical methods.[25–28]

By the DMRG method we study the systems with lengths $L = 32$ to 144 keeping $m \sim 25L$ density-matrix eigenstates. Note that an appropriate 1D array for the construction of the periodic boundary conditions (PBC) is necessary to obtain a highly accurate result (see Fig. 1 of Ref. 29). In this way, the largest discarded weight is $w_d \sim 2 \times 10^{-12}$ in the renormalization procedure and the central charge converges at least six digits as a function of m for a fixed system length. As examples, the DMRG results of c_1 and c_2 at $J_2/J_1 = 0$ and 0.2, where the system is in the TL-liquid phase, are shown in Table I for several system lengths. We can see that both of the quantities c_1 and c_2 converge very fast with increasing system length and they can be easily extrapolated to 1 in the thermodynamic limit. In fact, even for $L = 32$ the largest deviations from $c = 1$ are only 0.5 and 0.7% for c_1 and c_2, respectively. A finite-size correction is always smaller in c_1 than in c_2, so we make use only of c_1, namely Eq. (2), for the finite-size-scaling analysis below.

Now we demonstrate how one can estimate a critical point between the TL- and non-TL-liquid (or gapped) phases with Eq. (2). This is a good enduring test of Eq. (2) because the use of ΔS is no longer allowed due to the system-size-dependent frustration of the system in Eq. (4). This system belongs to the Gaussian universality class ($c = 1$) for the TL-liquid phase and $c < 1$ is expected for the gapped phase from the

TABLE I. System-size dependence of c_1 and c_2 obtained from Eqs. (2) and (3) for the 1D $S = \frac{1}{2}$ frustrated Heisenberg model.

	$J_2/J_1 = 0$		$J_2/J_1 = 0.2$	
L	c_1	c_2	c_1	c_2
32	1.005297	1.006916	1.001593	1.003206
64	1.002932	1.003335	1.000454	1.000856
96	1.002207	1.002386	1.000241	1.000420
128	1.001845	1.001945	1.000164	1.000260

renormalization in the massive region.[30] In Fig. 1 the DMRG results of c_1 are plotted as a function of J_2/J_1 for several system lengths. In the renormalization group the correction of the central charge is expressed as $c = 1 + \mathcal{O}(f^3)$, where f is the coupling constant of marginal operators,[31,32] so a "transition point" for a fixed system length may be given by a maximum of c_1. Actually, we find that all of those curves have a maximum at some point $(J_{2,\max}/J_1, c_{1,\max})$; on the left-hand side of the maximum point they become flatter and flatter and get closer to $c_1 = 1$ with increasing system length, whereas, on the right-hand side, c_1 drops down abruptly as a function of J_2/J_1. Hence, the maximum position must approach the critical point $J_2 = J_{2,c}$ as the system length increases and must reach there with $c_1 = 1$ in the thermodynamic limit, namely, $J_{2,\max} \to J_{2,c}$ and $c_{1,\max} \to 1$ as $L \to \infty$.

In Fig. 2(a) the maximum position $J_{2,\max}/J_1$ is plotted as a function of $1/L$ for systems with an even number of sites from $L = 32$ to 144. Although it oscillates due to the inconsistency between the periodicity of spin wave and the system length, i.e., system-size-dependent frustration, its amplitude decreases rapidly with increasing system length. Therefore, an extrapolation of $J_{2,\max}/J_1$ to the thermodynamic limit is practicable and we obtain $J_{2,c}/J_1 = 0.24112778$ by linear least-square fit with a weight function of $w(1/L) = L$ (without the weighting, $J_{2,c}/J_1 = 0.2414 \pm 0.001$). This value
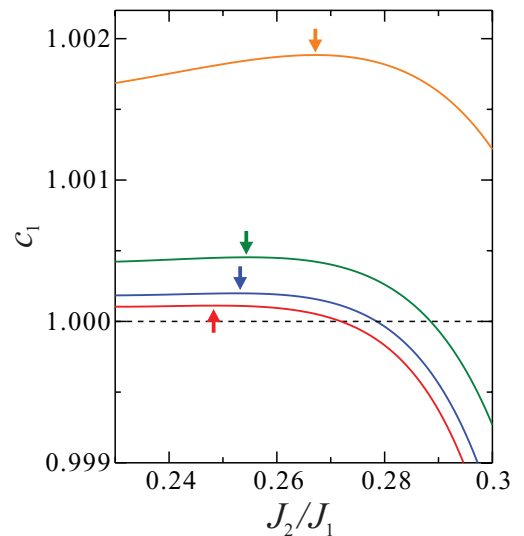

FIG. 1. (Color online) System-size dependence of c_1 as a function of J_2/J_1. The arrows indicate maximum positions $(J_{2,\max}/J_1, c_{1,\max})$. The system length is $L = 32$ (orange), 64 (green), 96 (blue), and 128 (red) from top to bottom.
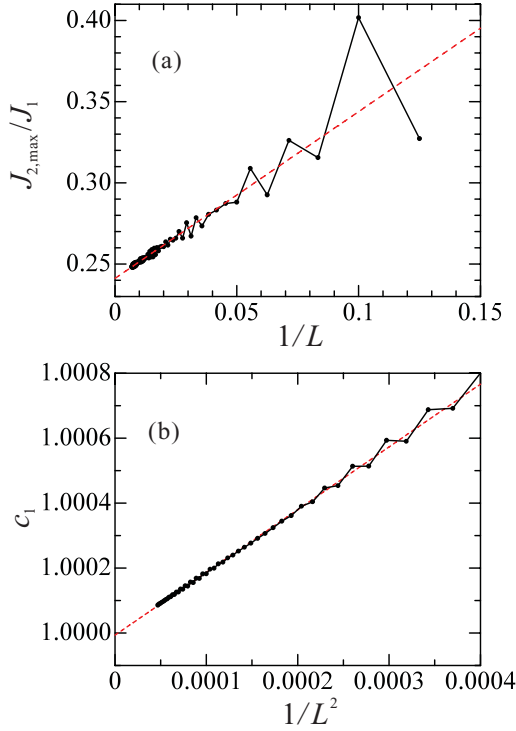
FIG. 2. (Color online) (a) Maximum position $J_{2,\text{max}}/J_1$ as a function of $1/L$ for systems with an even number of sites from $L = 32$ to 144. The red dashed line denotes a linear least-square fit with a weight function of $w(1/L) = L$. (b) Maximum height $c_{1,\text{max}}$ as a function of $1/L^2$ for systems with an even number of sites from $L = 32$ to 144. The red dashed line shows a simple linear fitting.

is consistent with the previous estimations.[22,23] Another thing to be examined is an extrapolation of the maximum height to the thermodynamic limit. The maximum height $c_{1,\text{max}}$ is plotted as a function of $1/L^2$ in Fig. 2(b). Interestingly, the data seem to be on a straight line at least for longer systems and we obtain $c = 0.999992824$ in the thermodynamic limit by a linear fitting. This implies that the central charge scales as

$$c_1 = 1 + \mathcal{O}(1/L^2). \tag{5}$$

This can be interpreted as the $\mathcal{O}(1/L^2)$ corrections originated from the $x = 4$ irrelevant fields in the CFT.[33] No sooner does J_2 moves away from $J_{2,c}$ than the system-size dependence of c_1 starts to deviate from Eq. (5). This means that the logarithmic corrections are completely eliminated only at this critical point. This is consistent with the fact that the effective Hamiltonian of system (4) is purely Gaussian only at the critical point. In this manner we can easily determine whether or not the logarithmic corrections are present for an arbitrary 1D quantum system.

B. Spinless fermions with nearest-neighbor repulsion

It is important to examine whether Eqs. (2) and (3) are applicable to itinerant fermion systems. Thus, as our second test we consider the 1D half-filled spinless fermions with nearest-neighbor repulsion. The Hamiltonian is given by

$$H = -t \sum_{\langle i,j \rangle} (c_i^\dagger c_j + \text{h.c.}) + V \sum_{\langle i,j \rangle} n_i n_j, \tag{6}$$

TABLE II. System-size dependence of c_1 and c_2 obtained from Eqs. (2) and (3) for the 1D half-filled spinless model with nearest-neighbor repulsion.

	$V/t = 0$		$V/t = 1.9$	
L	c_1	c_2	c_1	c_2
30	1.001119	1.002954	1.005450	1.007293
70	1.000199	1.000535	1.002542	1.002879
110	1.000082	1.000218	1.001818	1.001955
150	1.000041	1.000114	1.001467	1.001540

where $c_i^\dagger$ (c_i) is a creation (annihilation) operator of a spinless fermion and n_i ($=c_i^\dagger c_i$) is the corresponding number operator. The repulsive interaction V (>0) is assumed to act only between neighboring sites $\langle i,j \rangle$. The particle density is fixed at $n = 1/2$. This system can be mapped onto the exactly solvable Heisenberg XXZ chain and it is known that a transition between TL-liquid metallic and charge-density-wave insulating phases occurs at $V/t = 2 (\equiv V_c/t)$.

We study the systems with lengths $L = 30$ to 150 keeping $m \sim 40L$ density-matrix eigenstates. This way, the largest discarded weight is $w_d \sim 8 \times 10^{-12}$ in the renormalization procedure and the central charge converges at least seven digits as a function of m for a fixed system length. Table II shows the DMRG results of c_1 and c_2 at $V/t = 0$ and 1.9, where system (6) is in the TL-liquid phase, for several system lengths. In common with the case of the frustrated spin chain, the convergence of c_1 and c_2 with the system length is very fast and the deviation from $c = 1$ is always below 1% for $L > 30$. In Fig. 3 we plot the values of c_1 as a function of $1/L^2$ for some values of V/t. At $V/t = 0$, we see that c_1 is scaled by Eq. (5) and extrapolated to $c_1 = 1.00000062$ in the thermodynamic limit; however, for $V/t > 0$ Eq. (5) is no longer fulfilled due to the occurrence of the logarithmic corrections. As an example, the finite-size scaling of c_1 at $V/t = 2$, where the logarithmic corrections are maximum, is shown in the inset of Fig. 3.

So, let us check the behavior of c_1 on V/t near the critical point. In Fig. 4 the values of c_1 are plotted as a function of V/t for several system lengths. As seen in the frustrated spin chain,
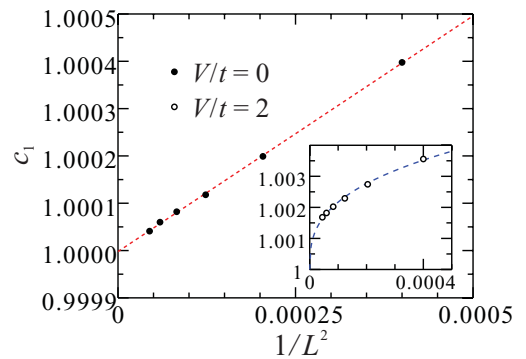

FIG. 3. (Color online) System-size dependence of c_1 as a function of $1/L^2$ for $V/t = 0$. The system lengths are taken at intervals of 20 sites from $L = 50$ to 150. The red dashed line shows a simple linear fitting. Inset: similar figure as the main one for $V/t = 2$. The blue dashed line is a guide to the eyes only.
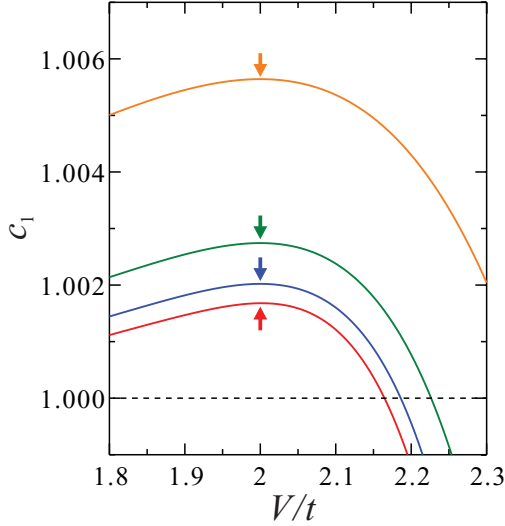
FIG. 4. (Color online) Finite-size-scaling analysis of c_1 as a function of V/t. The arrows indicate maximum positions ($V_{max}/t, c_{1,max}$). The system length is $L = 30$ (orange), 70 (green), 110 (blue), and 150 (red) from top to bottom.

each of the curves has a maximum at a point ($V_{max}, c_{1,max}$). Note that the peak position is exactly $V_{max}/t = 2$ for all system lengths. This is because the "critical point" is independent of the system length in this model [Eq. (6)]. Quite interestingly, it means that the critical point is not affected by the logarithmic corrections. Thus, we decide that Eqs. (2) and (3) are useful for a 1D itinerant system as well. Separately from this paper, it has been verified that this method is successfully applied to a 1D spinless fermion with boson affected hopping.[35]

Lastly, we mention that the TL parameter K_ρ, which is one of the most notable quantities to study the TL-liquid properties, can be estimated in a manner similar to above. The TL parameter is related to the charge-density fluctuation of the subsystem with length l, $F_L(l) = \langle (\sum_i n_i - \sum_i \bar{n}_i)^2 \rangle$ [$i \in$ subsystem], like[34]

$$\pi^2 F_L(l) = K_\rho \ln \left[\frac{L}{\pi} \sin \left(\frac{\pi l}{L} \right) \right] - \frac{(-1)^l A}{\left[\frac{L}{\pi} \sin \left(\frac{\pi l}{L} \right) \right]^{2K_\rho}} + f_1, \quad (7)$$

where A and f_1 are nonuniversal constants. The function $F_L(l)$ behaves similarly to $S_L(l)$ with l. Then, in the same way as Eq. (2) is derived, we easily obtain for $L \gg 1$

$$K_\rho \left[1 + (-1)^{\frac{L}{2}} 2A \left(\frac{\pi}{L} \right)^{2K_\rho} \right]$$
$$= \frac{\pi^2 \left[F_L \left(\frac{L}{2} - 2 \right) - F_L \left(\frac{L}{2} \right) \right]}{\ln \left[\cos \left(\frac{2\pi}{L} \right) \right]} \equiv K_\rho(L). \quad (8)$$

Since the $\mathcal{O}(L^{-2K_\rho})$ correction in Eq. (7) oscillates on alternate sites, the set of $F_L(\frac{L}{2})$ and $F(\frac{L}{2} - 2)$ is a more proper choice than that of $F_L(\frac{L}{2})$ and $F(\frac{L}{2} - 1)$. The values of $K_\rho(L)$ estimated from Eq. (8) at $V = 0$ as well as near the critical point are shown in Table III. With increasing L, $K_\rho(L)$ seems to approach the exact value

$$K_\rho = \frac{\pi}{2 \arccos[-V/(2t)]}. \quad (9)$$

TABLE III. System-size dependence of $K_\rho(L)$ obtained from Eqs. (8) for the 1D half-filled spinless model with nearest-neighbor repulsion. The extrapolated values to the thermodynamic limit ($L \to \infty$) and the exact values [Eq. (9)] are also shown.

L	$V = 0$	$V = 1.8$	$V = 1.9$
30	0.9926566	0.5212309	0.4940692
50	0.9973670	0.5476091	0.5202473
70	0.9986855	0.5587141	0.5314329
90	0.9992341	0.5648065	0.5376011
110	0.9995373	0.5683950	0.5417063
$L \to \infty$	1.0000593	0.5843504	0.5596052
Exact	1.0000000	0.5838163	0.5562247

We can easily perform the finite-size-scaling analysis with a fitting function $K_\rho(L) = K_\rho + aL^{-\gamma}$ ($1 \lesssim \gamma \leqslant 2$), where a and γ are fitting parameters. From Eq. (8), we know $a > 0$ ($a < 0$) for $L/2 =$ even (odd) and expect a simple relation $\gamma/2 \approx K_\rho$ if the logarithmic corrections are small. The fitting analyses are shown in Fig. 5. As expected, $\gamma/2 = 1$ is obtained at $V/t = 0$. Near the critical point, we have $\gamma/2 = 0.5312$ (0.4982) for $V/t = 1.8$ (1.9) and they have a kind of deviation from the exact values of K_ρ due to the existence of logarithmic corrections. Nonetheless, the extrapolated values are reasonably close to the exact ones (see Table III). The remaining error in the thermodynamic limit is only about 0.1% (0.6%) for $V/t = 1.8$ (1.9).

Here, we briefly comment on applying the open boundary conditions (OBC). Thus far the periodic boundary conditions are assumed; however, in general the OBC are more preferable in the DMRG study for accurate and convenient calculations. In this regard, with applying of the OBC the function $S_L(l)$ oscillates like Eq. (7) due to the Friedel oscillation and the analysis with Eq. (2) is unreasonable. If one can suppress
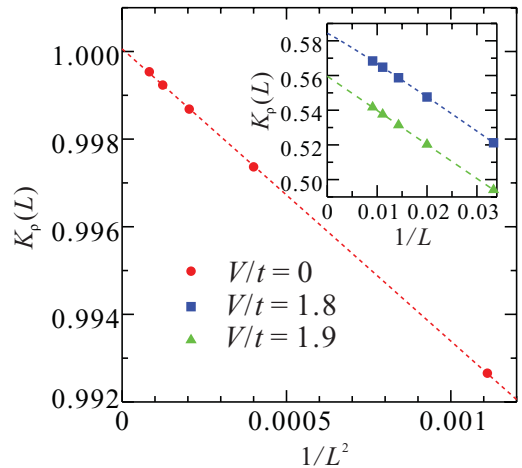

FIG. 5. (Color online) Finite-size-scaling analysis of $K_\rho(L)$ as a function of $1/L^2$ for $V/t = 0$. The system lengths are taken at intervals of 20 sites from $L = 30$ to 110. The red dashed line shows a simple linear fitting. Inset: finite-size-scaling analysis of $K_\rho(L)$ as a function of $1/L$ for $V/t = 1.8$ and 1.9. The blue and green dashed lines are fittings with function $K_\rho(L) = K_\rho + aL^{-\gamma}$. Through all the calculations $L/2$ is kept to be odd, and, therefore, $a < 0$ (see text).

the Friedel oscillation sufficiently at the center of the system, for example, by using the $\sin^2$-deformed OBC technique,[36,37] the central charge might be calculated by taking $S(\frac{L}{2})$ and $S(\frac{L}{2} - 2)$ as Eq. (8) even with the OBC.

IV. CONCLUSION

A numerical approach to calculate the central charge for a 1D quantum system using the entanglement entropy is proposed. This approach is applied to the frustrated spin chain and the half-filled spinless fermions with nearest-neighbor repulsion to check the validity. It is confirmed that the central charge is estimated very accurately for both the models, even with short system length. We also suggest a new method for determining the critical point between TL-liquid and gapped (or ordered) phases by using the proposed numerical approach. Furthermore, we demonstrate that the TL parameter can be calculated in a like manner as the central charge.

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