Extraction of topological information in Tomonaga-Luttinger liquids

Masaaki Nakamura[1] and Shunsuke C. Furuya[2]
[1]*Department of Physics, Ehime University Bunkyo-cho 2-5, Matsuyama, Ehime 790-8577, Japan*
[2]*Condensed Matter Theory Laboratory, RIKEN, Wako, Saitama 351-0198, Japan*

(Received 22 June 2018; revised manuscript received 24 December 2018; published 13 February 2019)

We discuss expectation values of the twist operator U appearing in the Lieb-Schultz-Mattis theorem (or the polarization operator for periodic systems) in excited states of the one-dimensional correlated systems $z_L^{(q,\pm)} \equiv \langle \Psi_{q/2}^{\pm} | U^q | \Psi_{q/2}^{\pm} \rangle$, where $|\Psi_p^{\pm}\rangle$ denotes the excited states given by linear combinations of momentum $2pk_F$ with parity ± 1. We found that $z_L^{(q,\pm)}$ gives universal values $\pm 1/2$ on the Tomonaga-Luttinger (TL) fixed point, and its signs identify the topology of the dominant phases. Therefore, this expectation value changes between $\pm 1/2$ discontinuously at a phase transition point with the U(1) or SU(2) symmetric Gaussian universality class. This means that $z_L^{(q,\pm)}$ extracts the topological information of TL liquids. We explain these results based on the free-fermion picture and the bosonization theory, and also demonstrate them in several physical systems.

DOI: 10.1103/PhysRevB.99.075128

I. INTRODUCTION

In many-body quantum systems, it is important to investigate structures of low-energy spectra such as the existence of energy gaps and the degeneracy of ground states. These structures of energy spectra characterize the physical properties of the systems such as metals or insulators, and dominant phases.

The Lieb-Schultz-Mattis (LSM) theorem plays an important role in the study of such properties in one-dimensional (1D) lattice systems [1–5]. In the LSM theorem, the possibility of opening an energy gap in a parity and translationally symmetric system is related to the orthogonality of a non-degenerate ground state in a finite-size system $|\Psi_0\rangle$ and a variational excited state $U^q|\Psi_0\rangle$. Here, U is the twist operator which creates the $O(1/L)$ excitation in a finite L size system. For fermion systems, that is defined by

$$U = \exp\left(\frac{2\pi i}{L}\sum_{j=1}^{L} j n_j\right), \tag{1}$$

where n_j is the density operator at site j. For spin systems, the twist operator is defined by replacing the density operator n_j by the spin operator S_j^z. It is well known that as a generalization of the original LSM theorem ($q = 1$), the necessary condition for the appearance of gapped states with q-fold degenerate ground states is given by $q(S - m) =$ integer where S and m are the spin and the magnetization per unit cell [4]. In this way

$$z_L^{(q)} = \langle \Psi_0 | U^q | \Psi_0 \rangle \tag{2}$$

is the essential index in the LSM theorem.

On the other hand, the same quantity $z_L^{(q)}$ is also introduced by Resta from an argument of electric polarization. He introduced $z_L^{(1)}$ to define the expectation value of the center-of-mass operator $\frac{1}{L}\sum_{j=1}^{L} j n_j$ in periodic systems [6–8]. This notion was also extended to q-fold degenerate systems [9]. It is well known that an insulator is distinguished from a conductor at zero temperature by its vanishing dc conductivity (Drude weight) [10], whereas, $z_L^{(q)}$ distinguishes not only metals and insulators, but also "topology" of insulators by its sign, such as band or Mott insulators. Thus $z_L^{(q)}$ plays the role of order parameters and also probes to detect topological phase transitions [11,12].

In this paper, we turn our attention to the following expectation value of U:

$$z_L^{(q,\pm)} = \langle \Psi_{q/2}^{\pm} | U^q | \Psi_{q/2}^{\pm} \rangle, \tag{3}$$

where $|\Psi_p^{\pm}\rangle$ denotes linear combinations of excited states with momenta $2pk_F$ and $-2pk_F$, and with parity $\mathcal{P}|\Psi_{q/2}^{\pm}\rangle = \pm|\Psi_{q/2}^{\pm}\rangle$. Here k_F is the Fermi momentum with $qk_F = n\pi$ (n: integer). This is as an extension of Eq. (2), but, as will be shown later, it extracts the topological information of 1D quantum systems at the limit of the Tomonaga-Luttinger (TL) fixed point as the universal values $z_L^{(q,\pm)} = \pm 1/2$, whereas $z_L^{(q)}$ becomes zero. This is essentially different from the property of $z_L^{(q)}$ whose sign is determined in the gapped fixed points.

This paper is organized as follows. In Sec. II, we discuss the properties of $z_L^{(q,\pm)}$ in the free fermions. In Sec. III, we discuss the interacting systems based on the TL model and bosonization of the twist operator. In Sec. IV, we demonstrate the properties in several physical systems based on the exact diagonalization (ED). Finally summary and discussions are given in Sec. V. Throughout this paper, the lattice constant and the Planck constant are set to be unity.

II. FREE-FERMION PICTURE

First, we consider the properties of Eq. (3) in free-fermion systems. It follows from the relation of the creation operators in the real and the momentum spaces, and the twist operator

$$U c_j^\dagger U^{-1} = c_j^\dagger e^{i(2\pi/L)j}, \quad U c_k^\dagger U^{-1} = c_{k+2\pi/L}^\dagger, \tag{4}$$

that U creates the momentum shift $\frac{2\pi}{L}$. This means that it creates momentum transfer $2k_F$ with respect to the ground

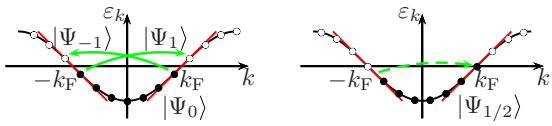

FIG. 1. Dispersion relations of the ground state $|\Psi_0\rangle$ and the excited states $|\Psi_p\rangle$ in finite-size systems. States with half-odd integers p are realized in the antiperiodic boundary condition, where the wave number $k = \frac{2\pi}{L}m$ with a half-odd integer m. In particular, excited states $|\Psi_{\pm 1/2}\rangle$ are realized as doubly degenerate ground states in the antiperiodic boundary condition. The momentum transfer of $|\Psi_{1/2}\rangle$ is regarded as $2k_F$ by 1/2 fermion.

state where the fermion states between $k = -k_F$ and $k = k_F$ are occupied. Now we introduce the following excited states:

$$|\Psi_p^{\pm}\rangle \equiv \frac{1}{\sqrt{2}}(|\Psi_{+p}\rangle \pm |\Psi_{-p}\rangle), \tag{5}$$

where $|\Psi_p\rangle$ is a state with a momentum $2pk_F$ (see Fig. 1). $|\Psi_p^{\pm}\rangle$ are eigenstates of the parity operation $\mathcal{P}|\Psi_p^{\pm}\rangle = \pm|\Psi_p^{\pm}\rangle$, since $\mathcal{P}|\Psi_p\rangle = |\Psi_{-p}\rangle$. The momentum is restricted by a condition $2pk_F = n\pi$ (n: integer), since the parity operation $\mathcal{P}$ ($\mathcal{P}c_i\mathcal{P}^{-1} = c_{L+1-i}$) commutes with the one-site shift operation $\mathcal{T}$ ($\mathcal{T}c_i\mathcal{T}^{-1} = c_{i+1}$) only when the eigenvalue of $\mathcal{T}$ is a real number ± 1. In this situation, the expectation value of the twist operator with an integer q becomes

$$\begin{aligned}\langle\Psi_p^{\pm}|\,U^q\,|\Psi_p^{\pm}\rangle &= \tfrac{1}{2}\,\langle\Psi_0|(U^q \pm U^{q-2p} \pm U^{q+2p} + U^q)|\Psi_0\rangle \\ &= \pm\tfrac{1}{2}\delta_{q,2p} \quad (L\to\infty).\end{aligned} \tag{6}$$

Here terms with the finite power of U vanish in the $L\to\infty$ limit due to the LSM theorem which insists that $|\Psi_0\rangle$ and $U^q|\Psi_0\rangle$ are orthogonal in the gapless state. Thus it turns out that $z_L^{(q,\pm)} = \pm 1/2$ and the signs identify parities of the wave function of the excited states (5) with $p = q/2$. Note that states with half-odd integers p are realized in antiperiodic boundary conditions, since the wave numbers are given by $k = \frac{2\pi}{L}m$ with half-odd integers m as shown in Fig. 1.

III. BOSONIZATION

Next, we demonstrate that the above property of $z_L^{(q,\pm)}$ is unchanged in interacting cases. To this end we consider the bosonization of the twist operator. In 1D systems, the low-energy excitations are described as TL liquids [13–15]. The Hamiltonian of the interacting fermions is given by the Gaussian model,

$$\mathcal{H}_{\rm TL} = v\int dx\left[\frac{\pi K}{2}\Pi^2 + \frac{1}{2\pi K}\left(\frac{\partial\phi}{\partial x}\right)^2\right], \tag{7}$$

where v and K are the sound velocity and the TL parameter, respectively. The phase fields satisfy $[\phi(x), \Pi(y)] = i\delta(x-y)$ and their mode expansions of the phase fields are given by

$$\phi(x) = \frac{i\pi}{L}\sum_{k\neq 0}\frac{1}{k}e^{-\alpha|k|/2-ikx}[\rho_+(k)+\rho_-(k)] + \frac{N\pi x}{L} + Q, \tag{8}$$

$$\Pi(x) = -\frac{1}{L}\sum_{k\neq 0}e^{-\alpha|k|/2-ikx}[\rho_+(k)-\rho_-(k)] - \frac{M}{L}, \tag{9}$$

with the cutoff α. The density operators satisfy the following commutation relation:

$$[\rho_r(-k), \rho_{r'}(k')] = r\frac{kL}{2\pi}\delta_{rr'}\delta_{kk'} \quad (r, r' = +, -), \tag{10}$$

and $\rho_+(-k)|\Psi_0\rangle = \rho_-(k)|\Psi_0\rangle = 0$ for $k > 0$. The zero mode satisfies the relation $[Q, M] = -i$. The effects of the interactions are renormalized into the TL parameter K, whereas $K = 1$ is for the free fermions. Usually, the low-energy Hamiltonian also includes a nonlinear term as $\mathcal{H} = \mathcal{H}_{\rm TL} + \frac{2g}{(2\pi\alpha)^2}\int_0 dx\,\cos[2q\phi(x)]$ which opens an energy gap when it is relevant in the renormalization group analysis. Therefore Hamiltonian (7) is realized just on the transition point with the Gaussian universality class ($g = 0$).

The center-of-mass operator is bosonized using the partial integration as

$$\frac{2\pi}{L}\sum_{j=1}^{L} jn_j \to \frac{2\pi}{L}\int_0^L dx\,x\frac{1}{\pi}\partial_x\phi(x) \tag{11}$$

$$= 2\phi(L) - N\pi - 2Q, \tag{12}$$

where we have ignored the $2k_F$-umklapp term. Then the normal ordered representation becomes [15] (see Appendix A)

$$U^q \to \mathcal{U}(q,K) \equiv \exp\{iq[2\phi(L) - N\pi - 2Q]\} \tag{13}$$

$$\simeq :\exp[i2q\phi(L)]: \left(\frac{2\pi\alpha}{L}\right)^{q^2K}. \tag{14}$$

If we set the cut-off parameter α to the order of the lattice constant ~ 1, this result describes the $O(1/L)$ excitation in the LSM theorem. This is also consistent with the conjecture $z_L^{(q)} \propto \langle\cos 2q\phi\rangle$ discussed in Ref. [11], since $z_L^{(q)}$ is a real number under the parity symmetry $\phi\to-\phi$. We can also confirm that the bosonized representation satisfies the relation (see Appendix A)

$$\mathcal{U}(q,K)\mathcal{U}(p,K) = \mathcal{U}(p+q,K). \tag{15}$$

For the interacting case with the forward scattering $K \neq 1$, it follows from the concept of TL liquids that the state with $2qk_F$ momentum $|\Psi_q\rangle$ is given by

$$|\Psi_q(K)\rangle = \mathcal{U}(q,K)\,|\Psi_0(K)\rangle\,, \tag{16}$$

where $|\Psi_0(K)\rangle$ is the ground state. Therefore, the relation for free fermions (6) is also applicable to the interacting case (7) only by a replacement $U^q \to \mathcal{U}(q,K)$. Thus within the low-energy approximation, the values $z_L^{(q,\pm)} = \pm 1/2$ turn out to be universal for the TL liquids with $K \neq 1$. This result does not depend on the detailed form of $\mathcal{U}(q,K)$ as long as relation (15) is satisfied.

In the conformal field theory (CFT), expectation values of one-point operators in finite-size systems are evaluated as [16,17] (see Appendix B)

$$\langle\mathcal{O}_i|\mathcal{O}_j(\sigma)|\mathcal{O}_i\rangle = C_{iji}\left(\frac{2\pi}{L}\right)^{x_j}, \tag{17}$$

where x_j is the scaling dimension of the jth operator, and C_{iji} is the operator product expansion (OPE) coefficient defined as

$$\mathcal{O}_i(\sigma_1)\mathcal{O}_j(\sigma_2) = \sum_k \frac{C_{ijk}}{|\sigma_1-\sigma_2|^{x_i+x_j-x_k}}\mathcal{O}_k(\sigma_2). \tag{18}$$

In the present case, the excited states $|\Psi^{\pm}_{q/2}\rangle$ are eigenstates of $\mathcal{O}_1(\sigma) \equiv :\cos[q\phi(\sigma)]:$ and $\mathcal{O}_2(\sigma) \equiv :\sin[q\phi(\sigma)]:$, respectively. In addition, $\mathcal{O}_3(\sigma) \equiv :\cos[2q\phi(\sigma)]:$ is related to the twist operator as $\mathcal{O}_3(L) \propto \mathcal{U}(q,K)$. The scaling dimensions are $x_1 = x_2 = q^2K/4$ and $x_3 = q^2K$. The OPE coefficients are $C_{131} = +1/2$ and $C_{232} = -1/2$ (see Appendix C). Then, the formula, Eq. (17), seems to explain Eq. (6), but the size dependence $(2\pi/L)^{x_3}$ remains. This discrepancy is because the bosonized operator $\mathcal{O}_3(L)$ is no longer a local field, so that Eq. (17) is not applicable to the present case.

IV. PHYSICAL SYSTEMS

A. The $S = 1/2$ J_1-J_2 spin chain

In the rest of this paper, we demonstrate the above argument in several models based on ED. As the first example, we consider the $S = 1/2$ antiferromagnetic Heisenberg chain with the next-nearest-neighbor exchanges,

$$\mathcal{H} = \sum_{i=1}^{L}[\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + \alpha \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2}]. \tag{19}$$

In this system, a phase transition between the gapless state and the dimer state occurs at $\alpha_c = 0.2411$ [18]. This critical point belongs to the universality class of the SU(2) symmetric Gaussian model, and is identified by the level crossing of the singlet-triplet excitation energies. These excited states correspond to $|\Psi^{\pm}_1\rangle$. The critical point can also be determined by the condition $z^{(2)}_L = 0$ [11,12] which is obtained by the ground-state expectation value of U^2 by ED for the $L = 28$ system, as shown in Fig. 2.

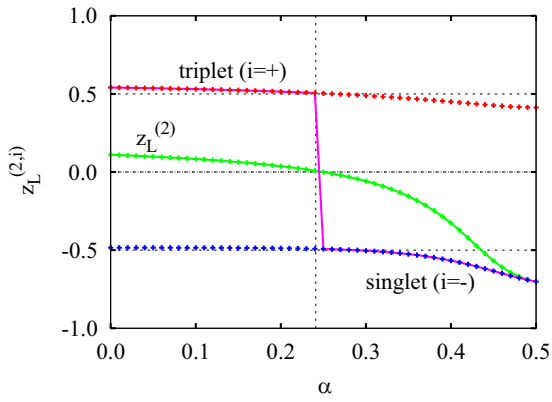

FIG. 2. $z^{(2,\pm)}_L$ of the $S = 1/2$ J_1-J_2 spin chain for the $L = 28$ system obtained by ED (red and blue lines). If we calculate the first excited state without classifying the Hilbert space by parity, the value change discontinuously between $\pm 1/2$ at the gapless-dimer transition point $\alpha_c = 0.2411$ (magenta line). On the other hand, $z^{(2)}_L$ changes continuously and becomes zero at α_c (green line). $z^{(2,\pm)}_L$ converges to $\pm 1/2$ for the gapless region, while to a finite value for the dimer region.

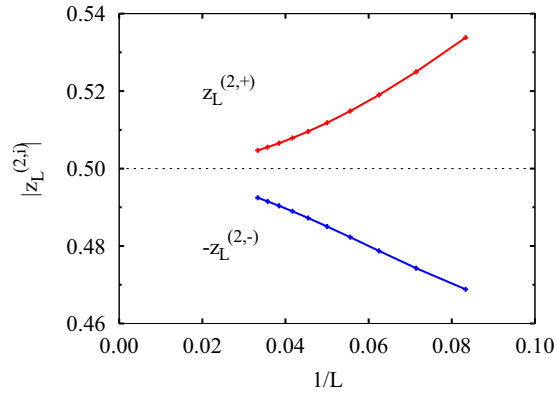

FIG. 3. System size dependence ($L = 12$–30) of $z^{(2,\pm)}_L$ of the $S = 1/2$ J_1-J_2 spin chain at the gapless-dimer transition point $\alpha_c = 0.2411$. This shows that $z^{(2,\pm)}_L$ has the size dependence $O(1/L)$, and approach to $\pm 1/2$ in the $L \to \infty$ limit.

Now we turn our attention to $z^{(2,\pm)}_L$ for the singlet $|\Psi^+_1\rangle$ and the triplet $|\Psi^-_1\rangle$ states corresponding to the dimer and the gapless states, respectively. According to the results of ED in Figs. 2 and 3, $z^{(2,\pm)}_L = \pm 1/2$ at the critical point $\alpha = \alpha_c$ with the size dependence $O(1/L)$. If we calculate the first excited state without classifying the Hilbert space by parity and/or spin-reversal symmetries, the expectation value changes discontinuously at α_c. For the gapless region $\alpha < \alpha_c$, the values $z^{(2,\pm)}_L = \pm 1/2$ are almost constant, while they deviate from $\pm 1/2$ for the dimer regions $\alpha > \alpha_c$. This indicates that for the gapped region $\langle\Psi_0|U^q|\Psi_0\rangle \neq 0$ due to the LSM theorem, so that Eq. (6) is not satisfied. For the Majumder-Gorsh point $\alpha = 0.5$ where the system is fully dimerized [19–22], the expectation values of U^2 with respect to the two states $|\Psi_0\rangle$ and $|\Psi^-_1\rangle$ give the same value $z^{(2,-)}_L = z^{(2)}_L \simeq -[\cos(2\pi/L)]^{L/2}$.

B. The $S = 1$ spin chain

The next example is the $S = 1$ Heisenberg chain with the single-ion anisotropy,

$$\mathcal{H} = \sum_{i=1}^{L}\left[\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + D\left(S^z_i\right)^2\right]. \tag{20}$$

This model undergoes a U(1) Gaussian-type phase transition from the Haldane-gap state [23,24] to the large-D (or trivial) state at $D_c = 0.968 \pm 0.001$ [25–27]. This transition point is determined by the level crossing of low-energy spectra of $|\Psi^{\pm}_{1/2}\rangle$ obtained with antiperiodic boundary conditions [28]. The twisted boundary conditions play a role to make artificial low-energy excitations that degenerate with the Haldane $|\Psi^-_{1/2}\rangle$ and large-D $|\Psi^+_{1/2}\rangle$ ground states, respectively. The transition point D_c can also be identified by $z^{(1)}_L = 0$ [29].

It follows from the results obtained by ED shown in Figs. 4 and 5, $z^{(1,\pm)}_L \pm 1/2$ with the size dependence $O(1/L)$. The excited states correspond to the Haldane ($|\Psi^-_{1/2}\rangle$) and the large-D ($|\Psi^+_{1/2}\rangle$) phases, respectively. Unlike the case of the $S = 1/2$ J_1-J_2 spin chain, $z^{(1,\pm)}_L$ deviates from $\pm 1/2$ away from D_c, because both regions $D \gtrless D_c$ are gapped states.

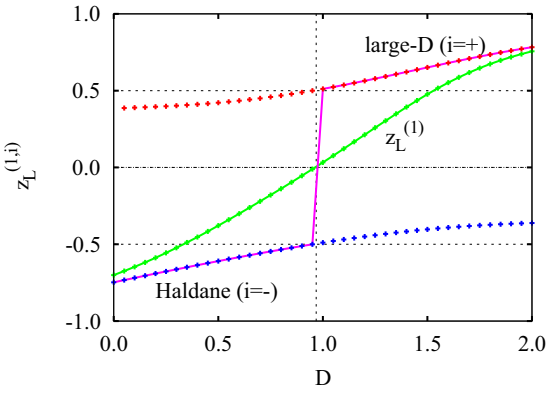

FIG. 4. $z_L^{(1,\pm)}$ of the $S = 1$ XXZ chain for the $L = 18$ system obtained by ED (red and blue lines). If we calculate the first excited state without classifying the Hilbert space by parity, the values change discontinuously between $\pm 1/2$ at the Haldane-large-D transition point $D_c = 0.968$ (magenta line). On the other hand, $z_L^{(1)}$ changes continuously and becomes zero at D_c (green line). $z_L^{(1,\pm)}$ do not converge to $\pm 1/2$ for the gapped regions $D \neq D_c$.

C. The extended Hubbard model

As an electron system, we consider the 1D extended Hubbard model at half-filling and zero magnetic field,

$$\mathcal{H} = \sum_{i=1}^{L} \left[-t \sum_{s=\uparrow,\downarrow} (c_{is}^{\dagger} c_{i+1,s} + \text{H.c.}) + U n_{i\uparrow} n_{i\downarrow} + V n_i n_{i+1} \right], \tag{21}$$

where c_{is} ($c_{is}^{\dagger}$) is the electron annihilation (creation) operator for spin $s = \uparrow, \downarrow$. The number operators are defined by $n_{is} \equiv c_{is}^{\dagger} c_{is}$ and $n_i \equiv n_{i\uparrow} + n_{i\downarrow}$. According to the analysis of the excitation spectra [30,31], the U(1) Gaussian transition in the charge part, and the SU(2) symmetric spin-gap transition take place independently near the $U = 2V$ line with $0 < U < U_c$, where U_c is the tricritical point. Therefore, there appear three phases around $U = 2V$. Those are spin-density-wave (SDW), bond-charge-density-wave (BCDW), and charge-density-wave (CDW) phases.

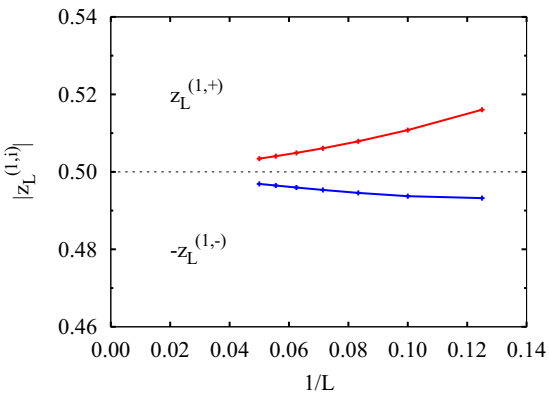

FIG. 5. System size dependence ($L = 8$–20) of $z_L^{(1,\pm)}$ of the $S = 1$ XXZ chain at the Haldane-large-D transition point $D_c = 0.968$. This shows that $z_L^{(1,\pm)}$ has the size dependence $O(1/L)$, and approach to $\pm 1/2$ in the $L \to \infty$ limit.

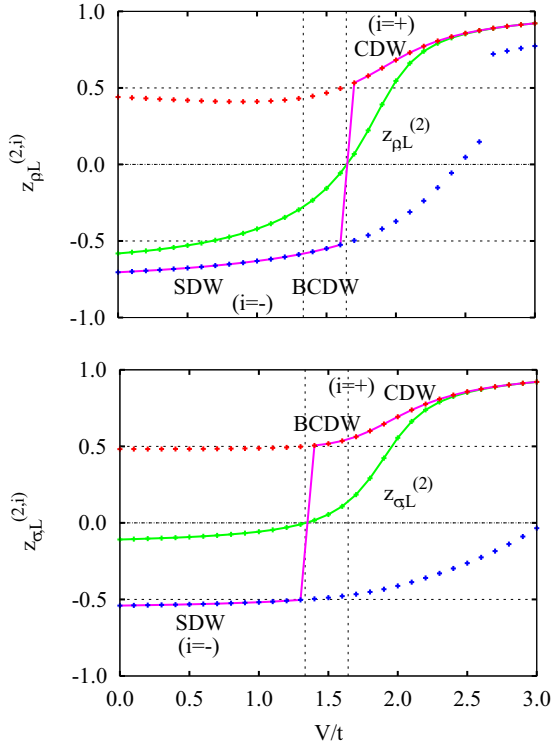

FIG. 6. $z_{\nu,L}^{(2,\pm)}$ of the extended Hubbard model for the charge ($\nu = \rho$) and the spin ($\nu = \sigma$) sectors for the $L = 14$ system at $U/t = 3$ obtained by ED (red and blue lines). At the BCDW-CDW (SDW-BCDW) boundary, we get $z_{\rho,L}^{(2,\pm)} = \pm 1/2$ ($z_{\sigma,L}^{(2,\pm)} = \pm 1/2$). The excited states $|\Psi_{\nu,1}^{\pm}\rangle$ are obtained under antiperiodic boundary conditions with wave number $k = \pi$ ($k = 0$) for $\nu = \rho$ ($\nu = \sigma$). If we calculate the first excited state without classifying the Hilbert space by parity, the value changes discontinuously between $\pm 1/2$ at these transition points (magenta line). On the other hand, $z_{\nu,L}^{(2)}$ changes continuously and becomes zero at the transition points (green line).

To apply our argument to the electron system, we introduce the twist operators for the charge and the spin sectors as [5]

$$U_\rho \equiv U_\uparrow U_\downarrow, \quad U_\sigma \equiv U_\uparrow U_\downarrow^{-1}, \tag{22}$$

where $U_s \equiv \exp[(2\pi i/L) \sum_{j=1}^{L} j n_{js}]$. Their ground-state expectation values $z_{\nu,L}^{(2)} \equiv \langle \Psi_0 | U_\nu | \Psi_0 \rangle$ ($\nu = \rho, \sigma$) give the BCDW-CDW ($z_{\rho,L}^{(2)} = 0$) and the SDW-BCDW ($z_{\sigma,L}^{(2)} = 0$) transition points, respectively [11]. In the present two-component case, the boson representation of U_ν is given by (14) where the phase fields for the charge ($\nu = \rho$) and the spin ($\nu = \sigma$) sectors are replaced as $\phi \to \phi_\nu/\sqrt{2}$.

As shown in Fig. 6, the expectation values of U_ν with respect to the excited states become $z_{\rho,L}^{(2,\pm)} = \pm 1/2$ at the BCDW-CDW transition point, and $z_{\sigma,L}^{(2,\pm)} = \pm 1/2$ at the SDW-BCDW transition point, respectively. Their system-size dependence at the critical points is $O(1/L)$ as shown in Fig. 7. The excited states $|\Psi_{\nu,1}^{\pm}\rangle$ are obtained under antiperiodic boundary conditions $c_{i+L,s}^{\dagger} = -c_{i,s}^{\dagger}$ with wave number $k = \pi$ ($k = 0$) for the charge $\nu = \rho$ (spin $\nu = \sigma$) sector [30,31].

In the present case, $z_{\rho,L}^{(2,\pm)}$ and $z_{\sigma,L}^{(2,\pm)}$ behave similarly to those of the $S = 1$ spin chain and the $S = 1/2$ J_1-J_2 spin chain, respectively, reflecting U(1) and SU(2) symmetries of the universality class of the transitions. The difference of the

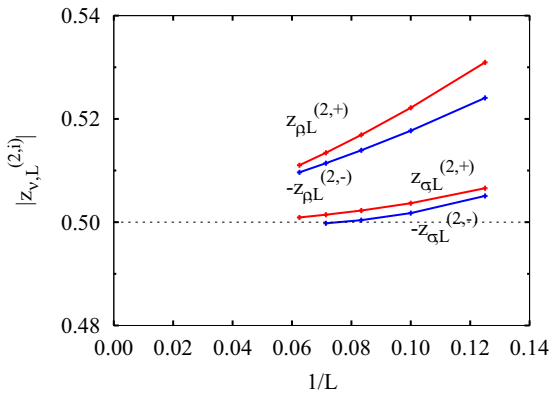

FIG. 7. System size dependence ($L = 8$–16) of $z_{\rho,L}^{(2,\pm)}$ of the extended Hubbard model at the BCDW-CDW boundary $V_c/t = 1.650$ and $z_{\sigma,L}^{(2,\pm)}$ at the SDW-BCDW boundary $V_c/t = 1.353$ at $U/t = 3$ [30,31]. This shows that $z_{\nu,L}^{(2,\pm)}$ has the size dependence $O(1/L)$, and approach to $\pm 1/2$ in the $L \to \infty$ limit.

signs of $z_{\sigma,L}^{(2,\pm)}$ and the $S = 1/2$ J_1-J_2 model is due to that of the coupling constant of the nonlinear terms g.

V. SUMMARY AND DISCUSSION

In summary, we have discussed the expectation value of the LSM-type twist operator U^q with respect to excited states $|\Psi_{q/2}^{\pm}\rangle$ that accompany momentum transfer qk_F. This takes the universal values $\pm 1/2$ in TL liquids, so that if the Hilbert space of these states is not classified by discrete symmetries, the expectation value changes discontinuously between these two values at the phase transition points that belong to the universality class of the U(1) or SU(2) symmetric Gaussian model. As a matter of fact, the behavior of $z_L^{(q,\pm)}$ is just like an "enhanced" version of $z_L^{(q)}$ which takes finite values with different signs at the two gapped fixed points but becomes zero at the transition point. However, the property of $z_L^{(q,\pm)}$ is essentially different from that of $z_L^{(q)}$ in terms that $z_L^{(q,\pm)}$ takes finite values on the limit of the gapless point. This property is applicable to detect these phase transitions and characterize the topology of the system. We have demonstrated these properties in the $S = 1/2$ J_1-J_2 spin chain, the $S = 1$ Heisenberg chain, and the extended Hubbard model.

In TL liquids, we cannot define order parameters as ground-state expectation values of operators, because the bosonized operator is always written in normal-ordered form. In other words, this is the consequence of an absence of long-range orders. Therefore, physical information in a TL liquid is usually characterized by the dominant exponents of the two-point correlation functions that show power-law decay. Contrary to this, our result indicates that we can enhance the order parameter $z_L^{(q)}$ and extract the physical information of TL liquids if the average is taken in terms of appropriate excited states.

In the present argument, the universal values $z_L^{(q,\pm)} = \pm 1/2$ in TL liquids do not depend on the detailed boson representation of $\mathcal{U}$ as long as relation (15) is satisfied. On the other hand, $z_L^{(q)} = 0$ on the Gaussian point is explained by the bosonized form (14) and the symmetry of the Gaussian point under the transformation $\phi \to \phi + \pi/2q$ which reverses the sign of the nonlinear term of the sine-Gordon model. In addition to this, there is small size dependence of the $z_L^{(q)} = 0$ point due to the approximation to the linearized dispersion relation of the TL model. Then, $\langle : e^{i2q\phi} : \rangle$ takes a finite value, and the size dependence mainly stems from the factor $(\frac{2\pi}{L})^{q^2K}$ of Eq. (14). Recently, the size dependence of $z_L^{(q)}$ away from the $z_L^{(q)} = 0$ point has been discussed [32]. For this case, effects of the marginal operator should be taken into account in the present case [33].

ACKNOWLEDGMENTS

M.N. acknowledges the Visiting Researcher's Program of the Institute for Solid State Physics, the University of Tokyo. The authors are grateful to M. Oshikawa for turning their attention to the current issue and for discussions. The authors also thank Y. Fuji, Y. Fukusumi, R. Kobayashi, Y. O. Nakagawa, S. Nishimoto, Y. Tada, and S. Todo for fruitful discussions. This work is supported by JSPS KAKENHI Grant No. 17K05580.

APPENDIX A: DERIVATION OF EQS. (14) AND (15)

We derive Eq. (14). By rescaling the density operators by the TL parameter and using the Campbell-Baker-Hausdorff formula $e^{A+B} = e^A e^B e^{-(1/2)[A,B]} = e^B e^A e^{(1/2)[A,B]}$, the normal-ordered representation of Eq. (13) is calculated as follows:

$$\mathcal{U}(1,K) \equiv \exp\{i[2\phi(L) - N\pi - 2Q]\} = \exp\left[-\sum_{n\neq 0}\frac{\sqrt{K}}{n}e^{-\alpha\pi|n|/L}[\tilde{\rho}_+(n) + \tilde{\rho}_-(n)] + iN\pi\right] \tag{A1}$$

$$= \underbrace{\exp\left[-\sum_{n>0}\frac{\sqrt{K}}{n}e^{-\alpha\pi|n|/L}[\tilde{\rho}_+(n) - \tilde{\rho}_-(-n)]\right]}_{\equiv\exp(i2\phi_>)}\underbrace{\exp\left[-\sum_{n<0}\frac{\sqrt{K}}{n}e^{-\alpha\pi|n|/L}[\tilde{\rho}_+(n) - \tilde{\rho}_-(-n)]\right]}_{\equiv\exp(i2\phi_<)}e^{iN\pi}$$

$$\times \exp\left\{\underbrace{-\frac{K}{2}\left[\sum_{n>0}\frac{1}{n}e^{-\alpha\pi|n|/L}[\tilde{\rho}_+(n) - \tilde{\rho}_-(-n)], \sum_{m<0}\frac{1}{m}e^{-\alpha\pi|m|/L}[\tilde{\rho}_+(m) - \tilde{\rho}_-(-m)]\right]}_{-\frac{K}{2}[i2\phi_>, i2\phi_<]\ (*)}\right\}, \tag{A2}$$

where we have redefined $\tilde{\rho}_\pm(n) \equiv \rho_\pm(p)$ with $p = \frac{2\pi}{L}n$. The marked part in Eq. (A2) becomes

$$\begin{aligned}(*) &= \exp\left(-\frac{K}{2}\sum_{n>0}\sum_{m<0}\frac{1}{nm}e^{-\alpha\pi(|n|+|m|)/L}\{[\tilde{\rho}_+(n)+\tilde{\rho}_-(-n)],[\tilde{\rho}_+(m)+\tilde{\rho}_-(-m)]\}\right)\\ &= \exp\left(-\frac{K}{2}\sum_{n>0}\frac{1}{n^2}e^{-\alpha 2\pi n/L}2n\right) = \exp\left(-K\sum_{n>0}\frac{1}{n}e^{-\alpha 2\pi n/L}\right) = \exp[K\log(1-e^{-\alpha 2\pi/L})]\\ &\simeq \left(\frac{2\pi\alpha}{L}\right)^K. \end{aligned} \tag{A3}$$

Therefore Eq. (A1) becomes

$$\begin{aligned}\mathcal{U}(1,K) &\simeq \left(\frac{2\pi\alpha}{L}\right)^K \exp(i2\phi_>)\exp(i2\phi_<)e^{iN\pi} \equiv \left(\frac{2\pi\alpha}{L}\right)^K :\exp[i(2\phi(L)-N\pi-2Q)]:\\ &\simeq \left(\frac{2\pi\alpha}{L}\right)^K :\exp[i2\phi(L)]:. \end{aligned} \tag{A4}$$

Thus we get Eq. (14). This satisfies Eq. (15) as follows:

$$\begin{aligned}\mathcal{U}(p,K)\mathcal{U}(q,K) &= \exp(i2p\phi_>)\exp(i2p\phi_<)e^{ipN\pi}\exp(i2q\phi_>)\exp(i2q\phi_<)e^{iqN\pi}\left(\frac{2\pi\alpha}{L}\right)^{(p^2+q^2)K}\\ &= \exp(i2p\phi_>)\exp(i2q\phi_>)\exp(i2p\phi_<)\exp(i2q\phi_<)e^{i(p+q)N\pi}\left(\frac{2\pi\alpha}{L}\right)^{(p^2+q^2)K}\exp(-[i2q\phi_>, i2p\phi_<])\\ &= \exp[i2(p+q)\phi_>]\exp[i2(p+q)\phi_<]e^{i(p+q)N\pi}\left(\frac{2\pi\alpha}{L}\right)^{(p^2+q^2+2pq)K}\\ &= \exp[i2(p+q)\phi_>]\exp[i2(p+q)\phi_<]e^{i(p+q)N\pi}\left(\frac{2\pi\alpha}{L}\right)^{(p+q)^2K}\\ &= \mathcal{U}(p+q,K). \end{aligned} \tag{A5}$$

APPENDIX B: ALTERNATIVE DERIVATION OF EQ. (17)

In Refs. [16,17], Eq. (17) has been derived based on the transfer-matrix method. Here we give an alternative derivation of this formula using only CFT. We consider an expectation value of an operator $\mathcal{O}_j$ in terms of excited states in the cylindrical coordinate as

$$z^{iji} \equiv {}_{\rm cyl}\langle\mathcal{O}_i|\mathcal{O}_j(\sigma)|\mathcal{O}_i\rangle_{\rm cyl}, \tag{B1}$$

where $|\mathcal{O}_i\rangle_{\rm cyl}$ is the highest weight state corresponding to the primary operator $\mathcal{O}_i(z,\bar{z})$. We assume that the operators are Hermitian $\mathcal{O}_i^\dagger = \mathcal{O}_i$. Then the counterpart of the two-dimensional plain $|\mathcal{O}_i\rangle$ and its conjugate state are defined as

$$|\mathcal{O}_i\rangle \equiv \lim_{z,\bar{z}\to 0} z^{-\Delta_i}\bar{z}^{-\bar{\Delta}_i}\mathcal{O}_i(z,\bar{z})|0\rangle, \tag{B2a}$$

$$\langle\mathcal{O}_i| \equiv \lim_{z,\bar{z}\to 0} z^{-\Delta_i}\bar{z}^{-\bar{\Delta}_i}\langle 0|\mathcal{O}_i(1/z,1/\bar{z}), \tag{B2b}$$

where $(\Delta_i, \bar{\Delta}_i)$ is the conformal dimension of $\mathcal{O}_i$. The above definitions satisfy the normalization condition $\langle\mathcal{O}_i|\mathcal{O}_i\rangle = 1$. We now define $|\mathcal{O}_i\rangle$ and $\langle\mathcal{O}_i|$ on a cylinder with length L as follows:

$$|\mathcal{O}_i\rangle_{\rm cyl} \equiv \lim_{w,\bar{w}\to-\infty}\left(\frac{L}{2\pi a z}\right)^{\Delta_i}\left(\frac{L}{2\pi a\bar{z}}\right)^{\bar{\Delta}_i}\mathcal{O}_i(w,\bar{w})|0\rangle, \tag{B3a}$$

$${}_{\rm cyl}\langle\mathcal{O}_i| \equiv \lim_{w,\bar{w}\to-\infty}\lim_{w'\to-w}\lim_{\bar{w}'\to-\bar{w}}\left(\frac{L}{2\pi a z}\right)^{\Delta_i}\left(\frac{L}{2\pi a\bar{z}}\right)^{\bar{\Delta}_i}\langle 0|\mathcal{O}_i(w',\bar{w}'), \tag{B3b}$$

where a is the lattice constant, and w, $\bar{w}$ and z, $\bar{z}$ are related by the conformal transformation,

$$w = \frac{L}{2\pi a}\ln z, \qquad \bar{w} = \frac{L}{2\pi a}\ln\bar{z}. \tag{B4}$$

The normalization between $|\mathcal{O}_i\rangle_{\rm cyl}$ and ${}_{\rm cyl}\langle\mathcal{O}_i|$ is confirmed as follows:

$$\begin{aligned}
{}_{\rm cyl}\langle\mathcal{O}_i|\mathcal{O}_i\rangle_{\rm cyl} &= \lim_{w,\bar{w}\to-\infty}\lim_{w'\to-w}\lim_{\bar{w}'\to-\bar{w}}\left(\frac{L}{2\pi a z}\right)^{2\Delta_i}\left(\frac{L}{2\pi a\bar{z}}\right)^{2\bar{\Delta}_i}\langle 0|\mathcal{O}_i(w',\bar{w}')\mathcal{O}_i(w,\bar{w})|0\rangle \\
&= \lim_{z,\bar{z}\to 0}\left(\frac{L}{2\pi a z}\right)^{2\Delta_i}\left(\frac{L}{2\pi a\bar{z}}\right)^{2\bar{\Delta}_i} \\
&\quad\times\lim_{z'\to 1/z}\lim_{\bar{z}'\to 1/\bar{z}}\left(\frac{L}{2\pi a z'}\right)^{-\Delta_i}\left(\frac{L}{2\pi a\bar{z}'}\right)^{-\bar{\Delta}_i}\left(\frac{L}{2\pi a z}\right)^{-\Delta_i}\left(\frac{L}{2\pi a\bar{z}}\right)^{-\bar{\Delta}_i}\langle 0|\mathcal{O}_i(z',\bar{z}')\mathcal{O}_i(z,\bar{z})|0\rangle \\
&= \lim_{z,\bar{z}\to 0}\left(\frac{1}{z}\right)^{2\Delta_i}\left(\frac{1}{\bar{z}}\right)^{2\bar{\Delta}_i}\frac{1}{(1/z)^{2\Delta_i}(1/\bar{z})^{2\bar{\Delta}_i}} \\
&= 1. \qquad \text{(B5)}
\end{aligned}$$

The expectation value of $\mathcal{O}_j(\sigma)=\mathcal{O}_j(w,\bar{w})$ with $w=\tau+i\sigma$, $\bar{w}=\tau-i\sigma$ in terms of $|\mathcal{O}_i\rangle_{\rm cyl}$ is calculated as follows:

$$\begin{aligned}
z^{iji} &= {}_{\rm cyl}\langle\mathcal{O}_i|\mathcal{O}_j(w,\bar{w})|\mathcal{O}_i\rangle_{\rm cyl} \\
&= \lim_{w'',\bar{w}''\to-\infty}\lim_{w'\to-w''}\lim_{\bar{w}'\to-\bar{w}'}\left(\frac{L}{2\pi a z''}\right)^{2\Delta_i}\left(\frac{L}{2\pi a\bar{z}''}\right)^{2\bar{\Delta}_i}\langle 0|\mathcal{O}_i(w',\bar{w}')\mathcal{O}_j(w,\bar{w})\mathcal{O}_i(w'',\bar{w}'')|0\rangle \\
&= \lim_{z'',\bar{z}''\to 0}\lim_{z'\to 1/z''}\lim_{\bar{z}'\to 1/\bar{z}''}\left(\frac{L}{2\pi a z''}\right)^{2\Delta_i}\left(\frac{L}{2\pi a\bar{z}''}\right)^{2\bar{\Delta}_i} \\
&\quad\times\left(\frac{L}{2\pi a z'}\right)^{-\Delta_i}\left(\frac{L}{2\pi a\bar{z}'}\right)^{-\bar{\Delta}_i}\left(\frac{L}{2\pi a z}\right)^{-\Delta_j}\left(\frac{L}{2\pi a\bar{z}}\right)^{-\bar{\Delta}_j}\left(\frac{L}{2\pi a z''}\right)^{-\Delta_i}\left(\frac{L}{2\pi a\bar{z}''}\right)^{-\bar{\Delta}_i} \\
&\quad\times\langle 0|\mathcal{O}_i(z',\bar{z}')\mathcal{O}_j(z,\bar{z})\mathcal{O}_i(z'',\bar{z}'')|0\rangle \\
&= \lim_{z'',\bar{z}''\to 0}\left(\frac{2\pi a}{L}\right)^{x_j}\frac{z^{\Delta_j}\bar{z}^{\bar{\Delta}_j}}{z''^{2\Delta_i}\bar{z}''^{2\bar{\Delta}_i}}\langle 0|\mathcal{O}_i(1/z'',1/\bar{z}'')\mathcal{O}_j(z,\bar{z})\mathcal{O}_i(z'',\bar{z}'')|0\rangle \qquad \text{(B6)} \\
&= \left(\frac{2\pi a}{L}\right)^{x_j}C_{iji}, \qquad \text{(B7)}
\end{aligned}$$

where $x_j=\Delta_j+\bar{\Delta}_j$ is the scaling dimension of $\mathcal{O}_j$, and C_{iji} is the OPE coefficient of the three-point function in Eq. (B6). Thus we get Eq. (17).

APPENDIX C: OPERATOR PRODUCT EXPANSION COEFFICIENTS

We calculate OPE coefficients involving the following operators:

$$\mathcal{O}_1(\sigma)=:\cos[q\phi(\sigma)]:,\quad \mathcal{O}_2(\sigma)=:\sin[q\phi(\sigma)]:,\quad \mathcal{O}_3(\sigma)=:\cos[2q\phi(\sigma)]:. \qquad \text{(C1)}$$

In a spin-1/2 chain, $\mathcal{O}_1$ and $\mathcal{O}_2$ correspond to the singlet state and the triplet state with $S^z=0$, respectively. $\mathcal{O}_3$ appears in the umklapp scattering term. The phase field is given by the holomorphic and the antiholomorphic parts as

$$\phi(z,\bar{z})=\frac{\sqrt{K}}{2}[\varphi(z)+\bar{\varphi}(\bar{z})]. \qquad \text{(C2)}$$

The vertex operators satisfy the following OPE rule for $z\simeq z'$:

$$:e^{i\alpha\varphi(z)}::e^{i\beta\varphi(z')}:\simeq(z-z')^{\alpha\beta}:e^{i(\alpha+\beta)\varphi(z')}:. \qquad \text{(C3)}$$

Then the OPE of $\mathcal{O}_2$, $\mathcal{O}_3$ is given by their most divergent terms as

$$\begin{aligned}
\mathcal{O}_2(z,\bar{z})\mathcal{O}_3(z',\bar{z}') &\simeq \frac{1}{4i}(:e^{iq\sqrt{K/4}\varphi(z)}::e^{iq\sqrt{K/4}\bar{\varphi}(\bar{z})}::e^{-iq\sqrt{K}\varphi(z')}::e^{-iq\sqrt{K}\bar{\varphi}(\bar{z}')}:-\text{H.c.}) \\
&\simeq \frac{1}{4i}\frac{1}{(z-z')^{q^2K/2}(\bar{z}-\bar{z}')^{q^2K/2}}(:e^{-iq\sqrt{K/4}\varphi(z')}::e^{-iq\sqrt{K/4}\bar{\varphi}(\bar{z}')}:-\text{H.c.}) \\
&= \frac{-1/2}{(z-z')^{q^2K/2}(\bar{z}-\bar{z}')^{q^2K/2}}\mathcal{O}_2(z',\bar{z}'). \qquad \text{(C4)}
\end{aligned}$$

Thus, we obtain $C_{232} = -1/2$. Similarly, we obtain $C_{131} = 1/2$ as

$$\mathcal{O}_1(z,\bar{z})\mathcal{O}_3(z',\bar{z}') \simeq \frac{1/2}{(z-z')^{q^2K/2}(\bar{z}-\bar{z}')^{q^2K/2}}\mathcal{O}_1(z',\bar{z}'). \tag{C5}$$

The process to obtain these universal values $C_{131} = 1/2$ and $C_{232} = -1/2$ is quite similar to that of Eq. (6).

[1] E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. (NY) **16**, 407 (1961).
[2] I. Affleck and E. H. Lieb, Lett. Math. Phys. **12**, 57 (1986).
[3] I. Affleck, Phys. Rev. B **37**, 5186 (1988).
[4] M. Oshikawa, M. Yamanaka, and I. Affleck, Phys. Rev. Lett. **78**, 1984 (1997).
[5] M. Yamanaka, M. Oshikawa, and I. Affleck, Phys. Rev. Lett. **79**, 1110 (1997).
[6] R. Resta, Phys. Rev. Lett. **80**, 1800 (1998).
[7] R. Resta and S. Sorella, Phys. Rev. Lett. **82**, 370 (1999).
[8] R. Resta, J. Phys.: Condens. Matter **12**, R107 (2000).
[9] A. A. Aligia and G. Ortiz, Phys. Rev. Lett. **82**, 2560 (1999).
[10] W. Kohn, Phys. Rev. **133**, A171 (1964).
[11] M. Nakamura and J. Voit, Phys. Rev. B **65**, 153110 (2002).
[12] M. Nakamura and S. Todo, Phys. Rev. Lett. **89**, 077204 (2002).
[13] F. D. M. Haldane, J. Phys. C **14**, 2585 (1981).
[14] T. Giamarchi, *Quantum Physics in One Dimension* (Oxford Science Press, Oxford, 2003).
[15] J. von Delft and H. Schoeller, Ann. Phys. (NY) **7**, 225 (1998).
[16] J. L. Cardy, Nucl. Phys. B **270**, 186 (1986).
[17] P. Reinicke, J. Phys. A **20**, 5325 (1987).
[18] K. Okamoto and K. Nomura, Phys. Lett. A **169**, 433 (1992).
[19] C. K. Majumder and D. K. Ghosh, J. Math. Phys. **10**, 1399 (1969).
[20] C. K. Majumder, J. Phys. C **3**, 911 (1970).
[21] I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, Phys. Rev. Lett. **59**, 799 (1987).
[22] I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, Commun. Math. Phys. **115**, 477 (1988).
[23] F. D. M. Haldane, Phys. Lett. A **93**, 464 (1983).
[24] F. D. M. Haldane, Phys. Rev. Lett. **50**, 1153 (1983).
[25] W. Chen, K. Hida, and B. C. Sanctuary, J. Phys. Soc. Jpn. **69**, 237 (2000).
[26] W. Chen, K. Hida, and B. C. Sanctuary, Phys. Rev. B **67**, 104401 (2003).
[27] W. Chen, K. Hida, and B. C. Sanctuary, J. Phys. Soc. Jpn. **77**, 118001 (2008).
[28] A. Kitazawa, J. Phys. A **30**, L285 (1997).
[29] M. Nakamura, E. J. Bergholtz, and J. Suorsa, Phys. Rev. B **81**, 165102 (2010).
[30] M. Nakamura, J. Phys. Soc. Jpn. **68**, 3123 (1999).
[31] M. Nakamura, Phys. Rev. B **61**, 16377 (2000).
[32] R. Kobayashi, Y. O. Nakagawa, Y. Fukusumi, and M. Oshikawa, Phys. Rev. B **97**, 165133 (2018).
[33] S. C. Furuya and M. Nakamura (unpublished).