Rigorous proof for the nonlocal correlation function in the transverse Ising model with ring frustration

Jian-Jun Dong, Zhen-Yu Zheng, and Peng Li*

College of Physical Science and Technology, Sichuan University, 610064, Chengdu, P. R. China and Key Laboratory of High Energy Density Physics and Technology of Ministry of Education, Sichuan University, 610064, Chengdu, P. R. China

(Received 24 March 2017; published 22 January 2018)

An unusual correlation function was conjectured by Campostrini *et al.* [Phys. Rev. E **91**, 042123 (2015)] for the ground state of a transverse Ising chain with geometrical frustration. Later, we provided a rigorous proof for it and demonstrated its nonlocal nature based on an evaluation of a Toeplitz determinant in the thermodynamic limit [J. Stat. Mech. (2016) 113102]. In this paper, we further prove that all the low excited energy states forming the gapless kink phase share the same asymptotic correlation function with the ground state. As a consequence, the thermal correlation function almost remains constant at low temperatures if one assumes a canonical ensemble.

DOI: 10.1103/PhysRevE.97.012133

I. INTRODUCTION

In the study of strongly correlated quantum systems, antiferromagnetic spin chains play an important role in demonstrating the strong quantum fluctuations that lead to rich and interesting physics [1,2]. In recent years, spin chains with designed boundary conditions have been attracting a lot of attention [3–6]. The simplest model providing many essential quantum physics of interest may be the Ising chain in a transverse field [7–11],

$$H_s = J\sum_{j=1}^{N}\sigma_j^x\sigma_{j+1}^x - h\sum_{j=1}^{N}\sigma_j^z, \tag{1}$$

with Pauli matrices $\sigma_j^\alpha(\alpha = x,z)$, exchange coupling J and transverse external field h. When appropriate boundary conditions are imposed with respect to geometrical frustration of spin arrangement, unusual properties may emerge [12–14]. In treating the transverse Ising ring with one-bond defect, Campostrini *et al.* [13] conjectured an unusual correlation function for the ground state based on numerical calculations. Later, in the context of the "a-cycle problem" [7], we analyzed the antiferromagnetically seamed chain with ring frustration [15], i.e., Eq. (1) with $J > 0$, $N \in$ Odd, and $\sigma_{j+N} = \sigma_j$, which is a translational invariant case considered in Ref. [13]. We rigorously proved the conjectured correlation function and showed its nonlocal nature. As disclosed by our rigorous solutions, there are $(2N-1)$ low-lying excited energy states similar to the ground state in the gapless kink phase ($h < J$) in the thermodynamic limit [15]. In this paper, we prove that the correlation functions of all the $(2N-1)$ low-lying excited energy states share the same asymptotic behavior with the ground state.

The organization of the paper is as follows. In Sec. II, the $2N$ low-lying energy states in the a-cycle problem of the Ising chain in a transverse field with ring frustration are reviewed. In Sec. III, we show how the correlation functions of the low excited states are represented by a set of Toeplitz determinants after tedious Wick contractions. In Sec. IV, we present a rigorous proof of a generalized theorem concerning the evaluation of the Toeplitz determinants in the thermodynamic limit. At last, the generalized theorem is used to work out the correlation functions in Sec. V.

II. THE 2N LOW-LYING ENERGY STATES

In this section, we briefly review the $2N$ low-lying energy states in the gapless kink phase that we obtained in our previous work [15].

First, by Jordan-Wigner transformation [16],

$$\sigma_j^+ = \left(\sigma_j^x + i\sigma_j^y\right)/2 = c_j^\dagger \exp\left(i\pi\sum_{l<j}c_l^\dagger c_l\right), \tag{2}$$

the system with ring geometry, Eq. (1), is mapped to a model of spinless fermions

$$H_f = Nh - 2h\sum_{j=1}^{N}c_j^\dagger c_j + J\sum_{j=1}^{N-1}(c_j^\dagger - c_j)(c_{j+1}^\dagger - c_{j+1}) - J\exp(i\pi M)(c_N^\dagger - c_N)(c_1^\dagger + c_1), \tag{3}$$

where $M = \sum_{l=1}^{N}c_l^\dagger c_l$ controls the parity of the fermion system. The last term in Eq. (3) can be regarded as a boundary constraint, which renders the fermions nonfree. Lieb *et al.* composed a free fermion model by loosing the boundary constraint and called it a c-cyclic problem, where c represents the free fermion operator. It is in contrast to the original spin Hamiltonian that is called the a-cyclic problem, where a represents the spin operator [7]. Now that we are exploring the effect of the ring frustration that is guaranteed by the boundary constraint, the fermion system Eq. (3) needs to be solved faithfully by full recovery of the exact degrees of freedom (DOF) of the spin system Eq. (1). The details were elaborated in our previous works [15,17]. In a nutshell, the

*lipeng@scu.edu.cn

fermion Hamiltonian Eq. (3) is solved in odd and even channels labeled by $M \in$ odd and $M \in$ even, respectively. But the total DOF of the two channels is twice as that of the original spin Hamiltonian Eq. (1). To restore the exact DOF of the original spin Hamiltonian, we have to remove the redundant DOF in each channel later [18].

Second, the Hamiltonian Eq. (3) is solved with the help of parity constraint, Fourier transformation $c_q = \frac{1}{\sqrt{N}}\sum_{j=1}^{N} c_j \exp(iqj)$, and Bogoliubov transformation ($q \neq 0$ and π),

$$\eta_q = u_q c_q - i v_q c_{-q}^\dagger, \tag{4}$$

with

$$u_q^2 = \frac{1}{2}\left[1+\frac{\epsilon(q)}{\omega(q)}\right],\ v_q^2 = \frac{1}{2}\left[1-\frac{\epsilon(q)}{\omega(q)}\right],$$
$$2u_q v_q = \frac{\Delta(q)}{\omega(q)}, \epsilon(q) = J\cos q - h, \Delta(q) = J\sin q, \tag{5}$$
$$\omega(q) = \sqrt{h^2+J^2-2hJ\cos q}.$$

In momentum space, the equivalence of the spin Hamiltonian and fermion Hamiltonian can be expressed as [19,20]

$$H_s = P^+ H_f^{(e)} P^+ \oplus P^- H_f^{(o)} P^-, \tag{6}$$

where $P^\pm = \frac{1}{2}[1 \pm \prod_{n=1}^{N}(1-2c_n^\dagger c_n)]$ are projectors on the subspaces with even or odd number of quasiparticles. Both $H_f^{(e)}$ and $H_f^{(o)}$ are fermion Hamiltonians. They are diagonalized in the even and odd channels respectively, which read

$$H_f^{(e)} = \epsilon(\pi)(2c_\pi^\dagger c_\pi - 1) + \sum_{q\in q^{(e)}, q\neq\pi} \omega(q)(2\eta_q^\dagger \eta_q - 1), \tag{7}$$
$$H_f^{(o)} = \epsilon(0)(2c_0^\dagger c_0 - 1) + \sum_{q\in q^{(o)}, q\neq 0} \omega(q)(2\eta_q^\dagger \eta_q - 1), \tag{8}$$

with

$$q^{(e)} = \left\{-\frac{N-2}{N}\pi, \ldots, -\frac{1}{N}\pi, \frac{1}{N}\pi, \ldots, \frac{N-2}{N}\pi, \pi\right\}, \tag{9}$$

$$q^{(o)} = \left\{-\frac{N-1}{N}\pi, \ldots, -\frac{2}{N}\pi, 0, \frac{2}{N}\pi, \ldots, \frac{N-1}{N}\pi\right\}. \tag{10}$$

The momentum values $q = 0$ and π play an important role in controlling the parity of valid states. In Eq. (6), $P^+ H_f^{(e)} P^+$ means the states with even number of fermions are valid, while $P^- H_f^{(o)} P^-$ means the ones with odd number of fermions are valid [18].

Then, in the kink phase ($h < J$), we write down the $2N$ low-lying energy states forming a gapless spectrum of band width $4h$. We group these states into four categories: (A) the *nondegenerate upper-most state with even parity*,

$$\left|E_\pi^{(e)}\right\rangle = |\phi^{(e)}\rangle, \tag{11}$$

(B) the *nondegenerate ground state with odd parity*,

$$\left|E_0^{(o)}\right\rangle = c_0^\dagger |\phi^{(o)}\rangle, \tag{12}$$

(C) the *doubly degenerate energy states with odd parity* [totally $(N-1)$ states],

$$\left|E_k^{(o)}\right\rangle = \eta_k^\dagger |\phi^{(o)}\rangle, \{k \in q^{(o)} | k \neq 0\}, \tag{13}$$

(D) the *doubly degenerate energy states with even parity* [totally $(N-1)$ states],

$$\left|E_k^{(e)}\right\rangle = \eta_k^\dagger c_\pi^\dagger |\phi^{(e)}\rangle, \{k \in q^{(e)} | k \neq \pi\}. \tag{14}$$

In the above states, the Bardeen-Cooper-Schrieffer-type wave functions

$$|\phi^{(o)}\rangle = \prod_{q\in q^{(o)}, 0<q<\pi} (u_q + i v_q c_q^\dagger c_{-q}^\dagger)|0\rangle, \tag{15}$$
$$|\phi^{(e)}\rangle = \prod_{q\in q^{(e)}, 0<q<\pi} (u_q + i v_q c_q^\dagger c_{-q}^\dagger)|0\rangle, \tag{16}$$

are vacuums corresponding to $H_f^{(e)}$ and $H_f^{(o)}$ respectively.

There is a rough but nice picture for these $2N$ low-lying energy states in a perturbative treatment ($h \ll J$), which gives the following translationally invariant energy states [15]:

$$|A_p\rangle = \frac{1}{\sqrt{2N}} \sum_{j=1}^{N} e^{-ipj}(|K(j),\leftarrow\rangle + |K(j),\rightarrow\rangle), \tag{17}$$
$$|B_p\rangle = \frac{1}{\sqrt{2N}} \sum_{j=1}^{N} e^{-ipj}(|K(j),\leftarrow\rangle - |K(j),\rightarrow\rangle), \tag{18}$$

where the classical one-kink states are

$$|K(j),\rightarrow\rangle = |\ldots, \leftarrow_{j-1}, \boxed{\rightarrow_j, \rightarrow_{j+1}}, \leftarrow_{j+2}, \ldots\rangle, \tag{19}$$
$$|K(j),\leftarrow\rangle = |\ldots, \rightarrow_{j-1}, \boxed{\leftarrow_j, \leftarrow_{j+1}}, \rightarrow_{j+2}, \ldots\rangle, \tag{20}$$

and the "quantum number" p reads

$$p = \left\{-\frac{N-1}{N}\pi, \ldots, -\frac{2}{N}\pi, 0, \frac{2}{N}\pi, \ldots, \frac{N-1}{N}\pi\right\}. \tag{21}$$

The correspondences between the exact states and the approximate ones are

$$\left|E_\pi^{(e)}\right\rangle \approx |B_0\rangle, \tag{22}$$
$$\left|E_k^{(o)}\right\rangle \approx |A_k\rangle, \tag{23}$$
$$\left|E_k^{(e)}\right\rangle \approx |B_{\pi-k}\rangle, \tag{24}$$
$$\left|E_0^{(o)}\right\rangle \approx |A_0\rangle. \tag{25}$$

III. TOEPLITZ DETERMINANT REPRESENTATION OF THE LONGITUDINAL CORRELATION FUNCTIONS

The two point longitudinal spin-spin correlation function for any arbitrary state $|\psi\rangle$ is defined as

$$C_{r,N}^{xx}(|\psi\rangle) = \langle\psi|\sigma_j^x \sigma_{j+r}^x|\psi\rangle = \langle\psi|B_j A_{j+1} \ldots B_{j+r-1} A_{j+r}|\psi\rangle, \tag{26}$$

where Jordan-Wigner transformation has been applied and notations $A_j = c_j^\dagger + c_j$ and $B_j = c_j^\dagger - c_j$ are introduced. Due to translational invariance, the correlation function depends on the distance r of two spins rather than the lattice position j. And because of the periodicity, we have a cyclic relation, $C^{xx}_{r,N}(|\psi\rangle) = C^{xx}_{N-r,N}(|\psi\rangle)$, for a translationally invariant state $|\psi\rangle$.

In treating the transverse Ising ring with one-bond defect, Campostrini *et al.* conjectured an unusual correlation function for the ground state [13]. It is exactly coincident with the one that we proved later for a transverse Ising chain with ring frustration [15], which reads

$$C^{xx}_{r,N}\left(\left|E^{(o)}_0\right\rangle\right) = (-1)^r\left(1 - \frac{h^2}{J^2}\right)^{1/4}(1-2\alpha), \qquad (27)$$

where $\alpha = r/N$. Since we have $C^{xx}_{r,N} = C^{xx}_{N-r,N}$ due to the ring geometry, the values of α can be restricted in the interval $0 < \alpha < 1/2$.

Meanwhile, one can easily find that the approximate states produced by the perturbative theory give a simpler correlation function,

$$C^{xx}_{r,N}(|A_p\rangle) = C^{xx}_{r,N}(|B_p\rangle) = (-1)^r(1-2\alpha). \qquad (28)$$

For the ground state $|E^{(o)}_0\rangle \approx |A_0\rangle$, Eq. (28) is a good approximation of Eq. (27) in the limit $h/J \to 0$. So one can tell the meaning of the two factors in Eq. (27): The factor $(1-2\alpha)$ captured by the perturbative theory comes from the superposition of $2N$ one-kink states, while the factor $(1-\frac{h^2}{J^2})$ reflects an attenuation due to the increasing of number of kinks in the exact states with the transverse field h increasing. And both factors are consequences of quantum fluctuations introduced by the transverse field term in the Hamiltonian.

However, can we safely say that the $2N$ exact states, Eq. (11)–(14), exhibit the same correlation function as depicted in Eq. (27)? To answer this question, two necessary steps need to be accomplished: (i) to deduce the Toeplitz determinant representation for all the correlation functions of the exact low-lying energy states and (ii) to prove a generalized theorem concerning the evaluation of the obtained Toeplitz determinant. The step (ii) will be carried out in the next section. We now accomplish the step (i) by demonstrating that the correlation functions of all the low-lying states can be cast into a uniform expression,

$$C^{xx}_{r,N}\left(\left|E^{(o/e)}_k\right\rangle\right) = \Theta(r,N,\beta_k,e^{ik}) = \begin{vmatrix} D_0 + \frac{2}{N}\beta_k & D_{-1} + \frac{2}{N}\beta_k e^{-ik} & \cdots & D_{1-r} + \frac{2}{N}\beta_k e^{i(1-r)k} \\ D_1 + \frac{2}{N}\beta_k e^{ik} & D_0 + \frac{2}{N}\beta_k & \cdots & D_{2-r} + \frac{2}{N}\beta_k e^{i(2-r)k} \\ \cdots & \cdots & \cdots & \cdots \\ D_{r-1} + \frac{2}{N}\beta_k e^{i(r-1)k} & D_{r-2} + \frac{2}{N}\beta_k e^{i(r-2)k} & \cdots & D_0 + \frac{2}{N}\beta_k \end{vmatrix}, \qquad (29)$$

where β_k will be specified later [see Eq. (39)]. The demonstration is presented in turn according to the categories of states (A)–(D) denoted by Eq. (11)–(14), respectively. Please note that the derivations are only valid for $h < J$.

A. The uppermost state, $|E^{(e)}_\pi\rangle$

This case turns out to be the simplest one. We can apply the Wick's theorem in respect to $|\phi^{(e)}\rangle$ in the usual way [7,10], which directly leads to a Toeplitz determinant,

$$C^{xx}_{r,N}\left(|E^{(e)}_\pi\rangle\right) = \langle\phi^{(e)}|B_jA_{j+1}\dots B_{j+r-1}A_{j+r}|\phi^{(e)}\rangle$$
$$= \begin{vmatrix} D^{(e)}_0 + \frac{2}{N} & D^{(e)}_{-1} + \frac{2}{N}e^{-i\pi} & \cdots & D^{(e)}_{1-r} + \frac{2}{N}e^{i(1-r)\pi} \\ D^{(e)}_1 + \frac{2}{N}e^{i\pi} & D^{(e)}_0 + \frac{2}{N} & \cdots & D^{(e)}_{2-r} + \frac{2}{N}e^{i(2-r)\pi} \\ \vdots & \vdots & \vdots & \vdots \\ D^{(e)}_{r-1} + \frac{2}{N}e^{i(r-1)\pi} & D^{(e)}_{r-2} + \frac{2}{N}e^{i(r-2)\pi} & \cdots & D^{(e)}_0 + \frac{2}{N} \end{vmatrix}, \qquad (30)$$

where the elements come from nonzero contractions, $\langle\phi^{(e)}|B_lA_m|\phi^{(e)}\rangle = D^{(e)}_{l-m+1} + \frac{2}{N}e^{i(l-m+1)\pi}$, and

$$D^{(e)}_n = \frac{1}{N}\sum_{q\,\in\,q^{(e)}} D(e^{iq})e^{-iqn}, \qquad (31)$$

$$D(e^{iq}) = \frac{-(J-he^{-iq})}{\sqrt{(J-he^{-iq})(J-he^{iq})}}. \qquad (32)$$

B. The ground state, $|E^{(o)}_0\rangle = c^\dagger_0|\phi^{(o)}\rangle$

For the ground state, we need to apply the Wick's theorem in respect to $|\phi^{(o)}\rangle$, but now there are extra operators, c_0 and $c^\dagger_0$, in the expression

$$C^{xx}_{r,N}\left(\left|E^{(o)}_0\right\rangle\right) = \langle\phi^{(o)}|c_0B_jA_{j+1}\dots B_{j+r-1}A_{j+r}c^\dagger_0|\phi^{(o)}\rangle. \qquad (33)$$

We can choose to eliminate the operators c_0 and $c_0^\dagger$ first by using contractions, $\langle\phi^{(o)}|c_0 c_0^\dagger|\phi^{(o)}\rangle = 1$ and $\langle\phi^{(o)}|A_m c_0^\dagger|\phi^{(o)}\rangle = -\langle\phi^{(o)}|B_m c_0^\dagger|\phi^{(o)}\rangle = \frac{1}{\sqrt{N}}$, to get an expression like

$$C^{xx}_{r,N}\left(\left|E_0^{(o)}\right\rangle\right) = \langle\phi^{(o)}|B_j A_{j+1}\ldots B_{j+r-1}A_{j+r}|\phi^{(o)}\rangle + \frac{2}{N}\langle\phi^{(o)}|B_{j+1}A_{j+2}\ldots B_{j+r-1}A_{j+r}|\phi^{(o)}\rangle + \frac{2}{N}\langle\phi^{(o)}|A_{j+1}B_{j+1}B_{j+2}A_{j+3}\ldots B_{j+r-1}A_{j+r}|\phi^{(o)}\rangle + \cdots. \tag{34}$$

Then by contractions $\langle\phi^{(o)}|B_l A_m|\phi^{(o)}\rangle = D^{(o)}_{l-m+1}$ with

$$D^{(o)}_n = \frac{1}{N}\sum_{q\,\in\, q^{(o)}} D(e^{iq})e^{-iqn}, \tag{35}$$

we can get

$$C^{xx}_{r,N}\left(\left|E_0^{(o)}\right\rangle\right) = \begin{vmatrix} D^{(o)}_0 & D^{(o)}_{-1} & \cdots & D^{(o)}_{1-r} \\ D^{(o)}_1 & D^{(o)}_0 & \cdots & D^{(o)}_{2-r} \\ \cdots & \cdots & \cdots & \cdots \\ D^{(o)}_{r-1} & D^{(o)}_{r-2} & \cdots & D^{(o)}_0 \end{vmatrix} + \begin{vmatrix} \frac{2}{N} & \frac{2}{N} & \cdots & \frac{2}{N} \\ D^{(o)}_1 & D^{(o)}_0 & \cdots & D^{(o)}_{2-r} \\ \cdots & \cdots & \cdots & \cdots \\ D^{(o)}_{r-1} & D^{(o)}_{r-2} & \cdots & D^{(o)}_0 \end{vmatrix} + \cdots + \begin{vmatrix} D^{(o)}_0 & D^{(o)}_{-1} & \cdots & D^{(o)}_{1-r} \\ D^{(o)}_1 & D^{(o)}_0 & \cdots & D^{(o)}_{2-r} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{2}{N} & \frac{2}{N} & \cdots & \frac{2}{N} \end{vmatrix}$$

$$= \begin{vmatrix} D^{(o)}_0 + \frac{2}{N} & D^{(o)}_{-1} + \frac{2}{N} & \cdots & D^{(o)}_{1-r} + \frac{2}{N} \\ D^{(o)}_1 + \frac{2}{N} & D^{(o)}_0 + \frac{2}{N} & \cdots & D^{(o)}_{2-r} + \frac{2}{N} \\ \vdots & \vdots & \vdots & \vdots \\ D^{(o)}_{r-1} + \frac{2}{N} & D^{(o)}_{r-2} + \frac{2}{N} & \cdots & D^{(o)}_0 + \frac{2}{N} \end{vmatrix}. \tag{36}$$

C. The $(N-1)$ odd parity states, $|E_k^{(o)}\rangle = \eta_k^\dagger|\phi^{(o)}\rangle$

The starting point is

$$C^{xx}_{r,N}\left(\left|E_k^{(o)}\right\rangle\right) = \langle\phi^{(o)}|\eta_k B_j A_{j+1}\ldots B_{j+r-1}A_{j+r}\eta_k^\dagger|\phi^{(o)}\rangle. \tag{37}$$

Likewise, the strategy is to eliminate the operators η_k and $\eta_k^\dagger$ first. Besides $\langle\phi^{(o)}|\eta_k\eta_k^\dagger|\phi^{(o)}\rangle = 1$, one can find the useful combined contractions,

$$\langle\phi^{(o)}|\eta_k B_l|\phi^{(o)}\rangle\langle\phi^{(o)}|A_m\eta_k^\dagger|\phi^{(o)}\rangle = \frac{\beta_k}{N}e^{ik(l-m+1)}, \tag{38}$$

$$\beta_k = -D(e^{-ik}). \tag{39}$$

So we can write down

$$2C^{xx}_{r,N}\left(\left|E_k^{(o)}\right\rangle\right) = \Big[\langle\phi^{(o)}|B_j A_{j+1}\ldots B_{j+r-1}A_{j+r}|\phi^{(o)}\rangle + \frac{2\beta_k}{N}\langle\phi^{(o)}|B_{j+1}A_{j+2}\ldots B_{j+r-1}A_{j+r}|\phi^{(o)}\rangle + \frac{2\beta_k e^{-ik}}{N}\langle\phi^{(o)}|A_{j+1}B_{j+1}B_{j+2}A_{j+3}\ldots B_{j+r-1}A_{j+r}|\phi^{(o)}\rangle + \cdots\Big] + \Big[\langle\phi^{(o)}|B_j A_{j+1}\ldots B_{j+r-1}A_{j+r}|\phi^{(o)}\rangle + \frac{2\beta_{-k}}{N}\langle\phi^{(o)}|B_{j+1}A_{j+2}\ldots B_{j+r-1}A_{j+r}|\phi^{(o)}\rangle + \frac{2\beta_{-k}e^{ik}}{N}\langle\phi^{(o)}|A_{j+1}B_{j+1}B_{j+2}A_{j+3}\ldots B_{j+r-1}A_{j+r}|\phi^{(o)}\rangle + \cdots\Big]. \tag{40}$$

The terms in Eq. (40) are grouped into two square brackets. Each group is of similar form of Eq. (34) and leads to a determinant like Eq. (36). Thus the correlation function can be represented by the sum of two Toeplitz determinants,

$$C^{xx}_{r,N}\left(\left|E_k^{(o)}\right\rangle\right) = \tfrac{1}{2}[\Gamma^{(o)}(r,N,\beta_k,e^{ik}) + \Gamma^{(o)}(r,N,\beta_{-k},e^{-ik})], \tag{41}$$

where

$$\Gamma^{(o)}(r,N,\beta_k,e^{ik}) = \begin{vmatrix} D_0^{(o)} + \frac{2}{N}\beta_k & D_{-1}^{(o)} + \frac{2}{N}\beta_k e^{-ik} & \cdots & D_{1-r}^{(o)} + \frac{2}{N}\beta_k e^{i(1-r)k} \\ D_1^{(o)} + \frac{2}{N}\beta_k e^{ik} & D_0^{(o)} + \frac{2}{N}\beta_k & \cdots & D_{2-r}^{(o)} + \frac{2}{N}\beta_k e^{i(2-r)k} \\ \cdots & \cdots & \cdots & \cdots \\ D_{r-1}^{(o)} + \frac{2}{N}\beta_k e^{i(r-1)k} & D_{r-2}^{(o)} + \frac{2}{N}\beta_k e^{i(r-2)k} & \cdots & D_0^{(o)} + \frac{2}{N}\beta_k \end{vmatrix}. \tag{42}$$

D. The $(N-1)$ even parity states, $|E_k^{(e)}\rangle = \eta_k^\dagger c_\pi^\dagger|\phi^{(e)}\rangle$

This is the most tedious case. Now the correlation function is given by

$$C_{r,N}^{xx}\big(\big|E_k^{(e)}\big\rangle\big) = \langle\phi^{(e)}|c_\pi \eta_k B_j A_{j+1}\dots B_{j+r-1}A_{j+r}\eta_k^\dagger c_\pi^\dagger|\phi^{(e)}\rangle. \tag{43}$$

First, to eliminate the operators c_π and $c_\pi^\dagger$, we apply the following relation in the contractions:

$$\langle\phi^{(e)}|c_\pi B_l|\phi^{(e)}\rangle\langle\phi^{(e)}|A_m c_\pi^\dagger|\phi^{(e)}\rangle - \langle\phi^{(e)}|c_\pi A_m|\phi^{(e)}\rangle\langle\phi^{(e)}|B_l c_\pi^\dagger|\phi^{(e)}\rangle = -\frac{2}{N}e^{i\pi\,(l-m+1)}, \tag{44}$$

to get an expression like

$$C_{r,N}^{xx}\big(\big|E_k^{(e)}\big\rangle\big) = \langle\phi^{(e)}|\eta_k B_j A_{j+1}\dots B_{j+r-1}A_{j+r}\eta_k^\dagger|\phi^{(e)}\rangle + \left(-\frac{2}{N}\right)\langle\phi^{(e)}|\eta_k B_{j+1}A_{j+2}\dots B_{j+r-1}A_{j+r}\eta_k^\dagger|\phi^{(e)}\rangle$$
$$+\left(-\frac{2e^{-i\pi}}{N}\right)\langle\phi^{(e)}|\eta_k A_{j+1}B_{j+1}B_{j+2}A_{j+3}\dots B_{j+r-1}A_{j+r}\eta_k^\dagger|\phi^{(e)}\rangle + \cdots. \tag{45}$$

Second, in each term of Eq. (45), the elimination of operators η_k and $\eta_k^\dagger$ can be done just like that has been done in Eq. (37). Eventually, we can arrive at

$$C_{r,N}^{xx}\big(\big|E_k^{(e)}\big\rangle\big) = \tfrac{1}{2}[\Gamma^{(e)}(r,N,\beta_k,e^{ik}) + \Gamma^{(e)}(r,N,\beta_{-k},e^{-ik})], \tag{46}$$

where

$$\Gamma^{(e)}(r,N,\beta_k,e^{ik}) = \begin{vmatrix} D_0^{(e)} + \frac{2}{N}\beta_k & D_{-1}^{(e)} + \frac{2}{N}\beta_k e^{-ik} & \cdots & D_{1-r}^{(e)} + \frac{2}{N}\beta_k e^{i(1-r)k} \\ D_1^{(e)} + \frac{2}{N}\beta_k e^{ik} & D_0^{(e)} + \frac{2}{N}\beta_k & \cdots & D_{2-r}^{(e)} + \frac{2}{N}\beta_k e^{i(2-r)k} \\ \cdots & \cdots & \cdots & \cdots \\ D_{r-1}^{(e)} + \frac{2}{N}\beta_k e^{i(r-1)k} & D_{r-2}^{(e)} + \frac{2}{N}\beta_k e^{i(r-2)k} & \cdots & D_0^{(e)} + \frac{2}{N}\beta_k \end{vmatrix}. \tag{47}$$

We shall concern the correlation functions in the thermodynamic limit $N \to \infty$. In this limit, we have

$$D_n^{(e)} = D_n^{(o)} = D_n \equiv \int_{-\pi}^{\pi} \frac{dq}{2\pi} D(e^{iq})\,e^{-iqn}, \tag{48}$$

so that the Toeplitz determinants, Eqs. (30), (36), (42), and (47), can be cast into the uniform expression Eq. (29).

IV. A GENERALIZED THEOREM

In our previous work [15], we proved a theorem for working out the correlation function Eq. (27) of the ground state, in which we see the term $\frac{2}{N}$ plays a crucial role even in the thermodynamic limit $N \to \infty$. Now that the term is generalized to $\frac{2\beta_k}{N}e^{ikn}$ as shown in Eq. (29), we need a general theorem for all the $2N$ low-lying energy states.

Theorem. Consider a general Toeplitz determinant coming from Eq. (29),

$$\Theta(r,N,x,e^{ik}) = \begin{vmatrix} \tilde{D}_0 & \tilde{D}_{-1} & \cdots & \tilde{D}_{1-r} \\ \tilde{D}_1 & \tilde{D}_0 & \cdots & \tilde{D}_{2-r} \\ \cdots & \cdots & \cdots & \cdots \\ \tilde{D}_{r-1} & \tilde{D}_{r-2} & \cdots & \tilde{D}_0 \end{vmatrix}, \tag{49}$$

with

$$\tilde{D}_n = D_n + \frac{x}{N}e^{ikn}, \tag{50}$$

where D_n is defined in Eq. (48). If the generating function $D(e^{iq})$ and $\ln D(e^{iq})$ are continuous on the unit circle $|e^{iq}| = 1$, then the behavior for large N *of* $\Theta(r,N,x,e^{ik})$ is given by $(1 \ll r < N)$

$$\Theta(r,N,x,e^{ik}) = \Delta_r\left(1 + \frac{xr}{N D\big(e^{-ik}\big)}\right), \tag{51}$$

where

$$\Delta_r = \mu^r \exp\left(\sum_{n=1}^{\infty} n d_{-n} d_n\right), \tag{52}$$

$$\mu = \exp\left[\int_{-\pi}^{\pi} \frac{dq}{2\pi} \ln D(e^{iq})\right], \tag{53}$$

$$d_n = \int_{-\pi}^{\pi} \frac{dq}{2\pi} e^{-iqn} \ln D(e^{iq}), \tag{54}$$

if the sum in Δ_r converges.

Proof. Let $e^{iq} = \xi$, and then we have $D_n = \int_{-\pi}^{\pi} \frac{dq}{2\pi} D(\xi)\xi^{-n}$ according to Eq. (48). Let us rewrite Eq. (49) as

$$\Theta(r,N,x,e^{ik}) = \begin{vmatrix} D_0 & D_{-1} & \cdots & D_{-r+1} \\ D_1 & D_0 & \cdots & D_{-r+2} \\ \cdots & \cdots & \cdots & \cdots \\ D_{r-1} & D_{r-2} & \cdots & D_0 \end{vmatrix} + \begin{vmatrix} \frac{x}{N} & D_{-1} & \cdots & D_{1-r} \\ \frac{x}{N}e^{ik} & D_0 & \cdots & D_{2-r} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{x}{N}e^{i(r-1)k} & D_{r-2} & \cdots & D_0 \end{vmatrix}$$

$$+\cdots+ \begin{vmatrix} D_0 & \frac{x}{N}e^{-ik} & \cdots & D_{2-r} \\ D_1 & \frac{x}{N} & \cdots & D_{2-r} \\ \cdots & \cdots & \cdots & \cdots \\ D_{r-1} & \frac{x}{N}e^{i(r-2)k} & \cdots & D_0 \end{vmatrix} + \begin{vmatrix} D_0 & D_{-1} & \cdots & \frac{x}{N}e^{i(1-r)k} \\ D_1 & D_0 & \cdots & \frac{x}{N}e^{i(2-r)k} \\ \cdots & \cdots & \cdots & \cdots \\ D_{r-1} & D_{r-2} & \cdots & \frac{x}{N} \end{vmatrix}$$

and compose a set of linear equations

$$\sum_{m=0}^{r-1} D_{n-m} x_m^{(r-1)} = \frac{x}{N} \mathrm{e}^{\mathrm{i}kn} , \ 0 \leqslant n \leqslant r-1. \tag{55}$$

These equations have an unique solution for $x_n^{(r-1)}$ if there exists a nonzero determinant:

$$\Delta_r \equiv \begin{vmatrix} D_0 & D_{-1} & \cdots & D_{1-r} \\ D_1 & D_0 & \cdots & D_{2-r} \\ \cdots & \cdots & \cdots & \cdots \\ D_{r-1} & D_{r-2} & \cdots & D_0 \end{vmatrix} \neq 0. \tag{56}$$

By Cramer's rule, we have the solution:

$$x_0^{(r-1)} = \frac{\begin{vmatrix} \frac{x}{N} & D_{-1} & \cdots & D_{1-r} \\ \frac{x}{N}e^{ik} & D_0 & \cdots & D_{2-r} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{x}{N}e^{i(r-1)k} & D_{r-2} & \cdots & D_0 \end{vmatrix}}{\Delta_r}, \tag{57}$$

$$x_1^{(r-1)} = \frac{\begin{vmatrix} D_0 & \frac{x}{N} & \cdots & D_{2-r} \\ D_1 & \frac{x}{N}e^{ik} & \cdots & D_{2-r} \\ \cdots & \cdots & \cdots & \cdots \\ D_{r-1} & \frac{x}{N}e^{i(r-1)k} & \cdots & D_0 \end{vmatrix}}{\Delta_r}, \tag{58}$$

$$\vdots$$

$$x_{r-1}^{(r-1)} = \frac{\begin{vmatrix} D_0 & D_{-1} & \cdots & \frac{x}{N} \\ D_1 & D_0 & \cdots & \frac{x}{N}e^{ik} \\ \cdots & \cdots & \cdots & \cdots \\ D_{r-1} & D_{r-2} & \cdots & \frac{x}{N}e^{i(r-1)k} \end{vmatrix}}{\Delta_r}. \tag{59}$$

So we arrive at

$$\Theta(r,N,x,e^{ik}) = \Delta_r + \Delta_r \sum_{n=0}^{r-1} e^{-ikn} x_n^{(r-1)}. \tag{60}$$

In our problem, Δ_r can be directly evaluated through the Szegö's theorem in the usual way,

$$\Delta_r = \mu^r \exp\left(\sum_{n=1}^{\infty} n d_{-n} d_n\right), \tag{61}$$

where

$$\mu = \exp\left[\int_{-\pi}^{\pi} \frac{dq}{2\pi} \ln D(e^{iq})\right], \tag{62}$$

$$d_n = \int_{-\pi}^{\pi} \frac{dq}{2\pi} e^{-iqn} \ln D(e^{iq}). \tag{63}$$

The nonlocal information is contained in the second term of Eq. (60), which leads to the main innovative part of this proof. Following the standard Wiener-Hopf procedure [21–23], we consider a generalization of Eq. (55),

$$\sum_{m=0}^{r-1} D_{n-m} x_m = y_n, \ 0 \leqslant n \leqslant r-1, \tag{64}$$

and define

$$x_n = y_n = 0 \quad \text{for} \quad n \leqslant -1 \quad \text{and} \quad n \geqslant r, \tag{65}$$

$$\begin{aligned} v_n &= \sum_{m=0}^{r-1} D_{-n-m} x_m \quad \text{for} \quad n \geqslant 1 \\ &= 0 \quad \text{for} \quad n \leqslant 0, \end{aligned} \tag{66}$$

$$u_n = \sum_{m=0}^{r-1} D_{r-1+n-m} x_m \quad \text{for} \quad n \geqslant 1$$
$$= 0 \quad \text{for} \quad n \leqslant 0. \tag{67}$$

We further introduce

$$D(\xi) = \sum_{n=-\infty}^{\infty} D_n \xi^n, \quad Y(\xi) = \sum_{n=0}^{r-1} y_n \xi^n,$$
$$V(\xi) = \sum_{n=1}^{\infty} v_n \xi^n, \quad U(\xi) = \sum_{n=1}^{\infty} u_n \xi^n,$$
$$X(\xi) = \sum_{n=0}^{r-1} x_n \xi^n. \tag{68}$$

Then from Eq. (64), we can get

$$D(\xi)X(\xi) = Y(\xi) + V(\xi^{-1}) + U(\xi)\xi^{r-1} \tag{69}$$

for $|\xi| = 1$.

Becuase both $D(\xi)$ and $\ln D(\xi)$ are continuous and periodic on the unit circle, $D(\xi)$ has a unique factorization, up to a multiplicative constant, in the form

$$D(\xi) = P^{-1}(\xi) Q^{-1}(\xi^{-1}), \tag{70}$$

for $|\xi| = 1$, such that $P(\xi)$ and $Q(\xi)$ are both analytic for $|\xi| < 1$ and continuous and nonzero for $|\xi| \leqslant 1$. We now substitute Eq. (70) into Eq. (69) and multiply with $Q(\xi^{-1})$ at both sides to get

$$P^{-1}(\xi)X(\xi) - [Q(\xi^{-1})Y(\xi)]_+ - [Q(\xi^{-1})U(\xi)\xi^{r-1}]_+$$
$$= [Q(\xi^{-1})Y(\xi)]_- + Q(\xi^{-1})V(\xi^{-1})$$
$$+ [Q(\xi^{-1})U(\xi)\xi^{r-1}]_-, \tag{71}$$

where the subscript $+(-)$ means that we should expand the quantity in the brackets into a Laurent series and keep only those terms where ξ is raised to a non-negative (negative) power. As a matter of fact, from the unique factorization Eq. (70), one can find that both $P(\xi)$ and $Q(\xi)$ are $+$ functions [21].

The left-hand side of Eq. (71) defines a function analytic for $|\xi| < 1$ and continuous on $|\xi| = 1$ and the right-hand side defines a function which is analytic for $|\xi| > 1$ and is continuous for $|\xi| = 1$. Taken together they define a function $E(\xi)$ analytic for all ξ except possibly for $|\xi| = 1$ and continuous everywhere. But these properties are sufficient to prove that $E(\xi)$ is an entire function which vanished at $|\xi| = \infty$ and thus, by Liouville's theorem, must be zero everywhere [21,22]. Therefore both the right-hand side and the left-hand side of Eq. (71) vanish separately and thus we have

$$X(\xi) = P(\xi)[Q(\xi^{-1})Y(\xi)]_+ + P(\xi)[Q(\xi^{-1})U(\xi)\xi^{r-1}]_+. \tag{72}$$

Furthermore, $U(\xi)$ can be neglected for large r [21–23]

$$X(\xi) \approx P(\xi)[Q(\xi^{-1})Y(\xi)]_+. \tag{73}$$

From Eqs. (60), (68) and (73), we have

$$\sum_{n=0}^{r-1} e^{-ikn} x_n^{(r-1)} = X(e^{-ik})$$
$$= P(e^{-ik})[Q(e^{ik})Y(e^{-ik})]_+, \tag{74}$$

Moreover, a comparison of Eq. (55) with Eq. (64) shows that

$$Y(e^{-ik}) = \frac{rx}{N}. \tag{75}$$

Together with Eq. (70), we get

$$X(e^{-ik}) = \frac{xr}{N} P(e^{-ik})[Q(e^{ik})]_+$$
$$= \frac{xr}{N} P(e^{-ik}) Q(e^{ik}) = \frac{xr}{N D(e^{-ik})}. \tag{76}$$

From Eqs. (60), (74), and (76), we finally arrive at

$$\Theta(r,N,x,e^{ik}) = \Delta_r \left(1 + \frac{xr}{N D(e^{-ik})}\right). \tag{77}$$

■

V. EVALUATION OF THE CORRELATION FUNCTIONS AND CONCLUSION

Now we need to work out Δ_r in Eq. (77) that is defined in Eq. (61). For the gapless kink phase $h < J$, we have

$$D(e^{iq}) = -\sqrt{\frac{1 - \lambda e^{-iq}}{1 - \lambda e^{iq}}}, \tag{78}$$

where we have defined $\lambda = \frac{h}{J}$. Furthermore, because $0 < \lambda < 1$, we use the formula

$$\ln(1 - \lambda e^{iq}) = -\sum_{m=1}^{\infty} \frac{1}{m} (\lambda e^{iq})^m \tag{79}$$

to get

$$\ln D(e^{iq}) = i\pi - \frac{1}{2}\ln(1 - \lambda e^{iq}) + \frac{1}{2}\ln(1 - \lambda e^{-iq})$$
$$= i\pi + \frac{1}{2}\sum_{m=1}^{\infty} \frac{\lambda^m}{m} e^{iqm} - \frac{1}{2}\sum_{m=1}^{\infty} \frac{\lambda^m}{m} e^{-iqm}.$$

Thus we have

$$\mu = \exp\left[\int_{-\pi}^{\pi} \frac{dq}{2\pi} \ln D(e^{iq})\right] = -1,$$

and for $n > 0$

$$d_n = -\frac{\lambda^n}{2n}, \quad d_{-n} = \frac{\lambda^n}{2n}.$$

Then we found

$$\sum_{n=1}^{\infty} n d_n d_{-n} = -\frac{1}{4}\sum_{n=1}^{\infty} \frac{1}{n}\lambda^{2n} = \frac{1}{4}\ln(1 - \lambda^2). \tag{80}$$

By Szegö's theorem Eq. (61) we can get

$$\Delta_r = (-1)^r \left(1 - \frac{h^2}{J^2}\right)^{1/4}. \tag{81}$$

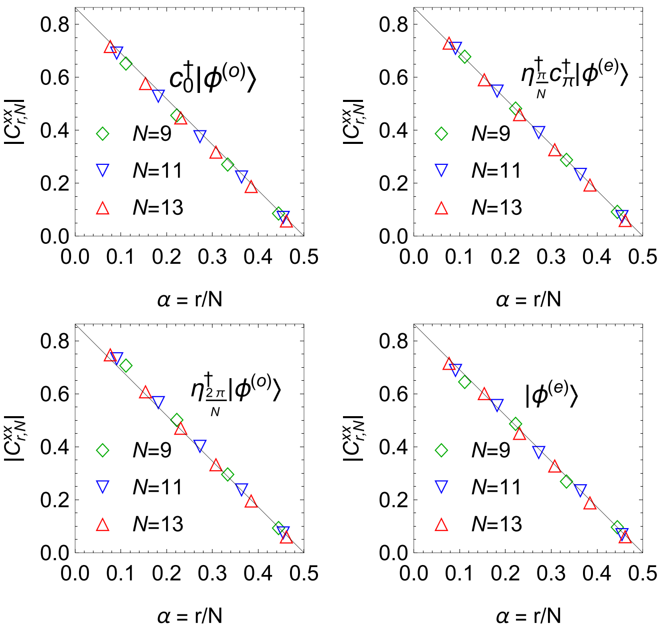

FIG. 1. The correlation functions for the ground state $|E_0^{(o)}\rangle = c_0^\dagger|\phi^{(o)}\rangle$, the first excited state $|E^{(e)}_{\frac{\pi}{N}}\rangle = \eta^\dagger_{\frac{\pi}{N}} c^\dagger_\pi|\phi^{(e)}\rangle$, the second excited state $|E^{(o)}_{\frac{2\pi}{N}}\rangle = \eta^\dagger_{\frac{2\pi}{N}}|\phi^{(o)}\rangle$, and the upper-most state $|E^{(e)}_\pi\rangle = |\phi^{(e)}\rangle$. The black straight line in each figure is the analytic result from Eq. (83) at $J/h = 1.5$. The colored dingbat data are exact diagonalization solutions of the original spin Hamiltonian Eq. (1) for $N = 9,11,13$.

Finally, we can evaluate the general Toeplitz determinant $\Theta(r,N,\beta_k,e^{ik})$ in Eq. (29) and get

$$\Theta(r,N,\beta_k,e^{ik}) = (-1)^r\left(1-\frac{h^2}{J^2}\right)^{1/4}\left(1-\frac{2r}{N}\right) \qquad (82)$$

for large-enough r and N. And by substituting Eq. (82) into Eqs. (30), (36), (41), and (46), we find that all the correlation functions of the $2N$ low-lying energy states exhibit the same asymptotic behavior,

$$C^{xx}_{r,N}\left(\left|E_k^{(o/e)}\right\rangle\right) = (-1)^r\left(1-\frac{h^2}{J^2}\right)^{1/4}(1-2\alpha),$$
$$(k \in q^{(o)} \cup q^{(e)}). \qquad (83)$$

It is worthwhile to note that the result is independent of wave number k.

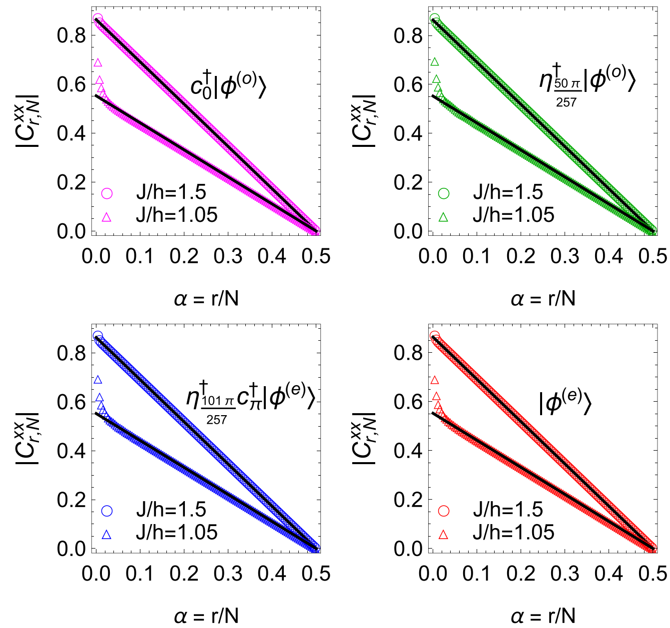

FIG. 2. The correlation functions for a system of $N = 257$ at $J/h = 1.05$ and 1.5 for several selected low-lying energy states, $c_0^\dagger|\phi^{(o)}\rangle$, $\eta^\dagger_{\frac{50\pi}{257}} c^\dagger_\pi|\phi^{(o)}\rangle$, $\eta^\dagger_{\frac{101\pi}{257}}|\phi^{(e)}\rangle$, and $|\phi^{(e)}\rangle$. The black straight line in each figure is the analytic result from Eq. (83). The colored dingbat data are direct evaluations of the Toeplitz determinants in Eq. (30), (36), (41), and (46). One can see that the data accurately agree with the analytic formula.

To confirm that the analytic result is correct, we compare it with the exact diagonalization solutions of the original spin Hamiltonian Eq. (1) for $N = 9,11,13$ and several low-lying energy states in Fig. 1. In Fig. 2, we compare it with the numerical data that are obtained by direct evaluation through the Toeplitz determinants. We see that the numerical data obey the asymptotic behavior accurately.

If assuming a canonical ensemble, then one would agree that the $2N$ low-lying energy states dominate the system's properties at low temperatures ($T \ll 4h/k_B$, where k_B is the Boltzmann constant) and then arrive at a conclusion that the thermal correlation function is inert to temperature.

ACKNOWLEDGMENTS

This work is supported by the NSFC under Grant No. 11074177 and SRF for ROCS SEM (Grant No. 20111139-10-2).

[1] N. Nagaosa, *Quantum Field Theory in Strongly Correlated Electronic System* (Springer, Berlin, 1999).
[2] S. Sachdev, *Quantum Phase Transitions* (Cambridge University Press, Cambridge, 2001).
[3] S. A. Owerre and J. Nsofini, Europhys. Lett. **110**, 47002 (2015).
[4] S. A. Owerre and M. B. Paranjape, Phys. Lett. A **378**, 3066 (2014).
[5] M. Okuyama, Y. Yamanaka, H. Nishimori, and M. M. Rams, Phys. Rev. E **92**, 052116 (2015).
[6] U. Marzolino, S. M. Giampaolo, and F. Illuminati, Phys. Rev. A **88**, 020301(R) (2013).
[7] E. H. Lieb, T. D. Schultz, and D. C. Mattis, Ann. Phys. **16**, 407 (1961).
[8] P. Pfeuty, Ann. Phys. **57**, 79 (1970).
[9] E. Barouch and B. McCoy, Phys. Rev. A **3**, 786 (1971).
[10] S. Suzuki, J. I. Bikas, and K. Chakrabarti, *Quantum Phase and Transitions in Transverse Ising Models*, Lecture Notes in Physics Vol. 862 (Springer, Berlin, 2013).

[11] A. Dutta, G. Aeppli, B. K. Chakrabarti, U. Divakaran, T. F. Rosenbaum, and D. Sen, *Quantum Phase Transitions in Transverse Field Spin Models: From Statistical Physics to Quantum Information* (Cambridge University Press, Cambridge, 2015).
[12] G. G. Cabrera and R. Jullien, Phys. Rev. B **35**, 7062 (1987).
[13] M. Campostrini, A. Pelissetto, and E. Vicari, Phys. Rev. E **91**, 042123 (2015).
[14] M. Campostrini, A. Pelissetto, and E. Vicari, J. Stat. Mech. (2015) P11015.
[15] J.-J. Dong, P. Li, and Q.-H. Chen, J. Stat. Mech. (2016) 113102.
[16] P. Jordan and E. Wigner, Z. Phys. **47**, 631 (1928).
[17] J.-J. Dong and P. Li, Mod. Phys. Lett. B **31**, 1750061 (2017).
[18] T. D. Schultz, D. C. Mattis, and E. H. Lieb, Rev. Mod. Phys. **36**, 856 (1964).
[19] J. Dziarmaga, Phys. Rev. Lett. **95**, 245701 (2005).
[20] F. Franchini, *An Introduction to Integrable Techniques for One-Dimensional Quantum Systems*, Springer Briefs in Mathematical Physics Vol. 16 (Springer, Berlin, 2017).
[21] B. M. McCoy, *Advanded Statistical Mechanics* (Oxford University Press, Oxford, 2010).
[22] B. M. McCoy and T. T. Wu, *The Two-Dimensional Ising Model* (Havard University Press, Cambridge, MA, 1973).
[23] T. T. Wu, Phys. Rev. **149**, 380 (1966).