Ring frustration and factorizable correlation functions of critical spin rings

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Tackling the critical transverse Ising ring with or without ring frustration, we establish the concept of nonlocality in a many-body system in the thermodynamic limit by calculating the nonlocal factors embedded in the factorizable correlation function. Through this exactly solvable prototype, we clearly show the intriguing difference between the periodic chains with odd and even numbers of lattice sites even in the thermodynamic limit. In the context of nonlocality, we also address the important application of finite-size scaling analysis by numerically working out the nonlocal factors of the isotropic XY model and the spin-1/2 Heisenberg model.

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I. INTRODUCTION

In quantum spin systems, highly entangled ground state can arise from geometrical frustration [1] as well as quantum frustration [2]. Quantum frustration means the frustrationlike effect may arise due to noncommutativity and entanglement in the quantum systems without geometrical frustration [3–7]. But it is usually not easy to discern the contributions of the two different sources [5]. Recently, the effect of ring frustration aroused much attention due to the exotic ground state it induced [8–16]. A nonlocal factor in its correlation function can be extracted, which represents the pure effect of geometrical frustration [13–15]. Ring frustration is a kind of geometrical frustration that occurs for a closed chain (Fig. 1), in which no unique Ising-like state can prevail in the ground state and minimize the system's energy alone. Unlike the usual local geometric frustration on the triangular or Kagomé lattices, the ring frustration is of a nonlocal nature in that (i) one must walk all the way round the ring to make sure of the presence of spin frustration, i.e., the frustration is somewhat *weak* [16] and (ii) it can significantly change the bulk property of the low-energy states [13,14]. Frustrations in spin rings have also been studied in [17–19].

On the other hand, the concept of thermodynamic limit resides in the central part of statistical mechanics, with which the critical phenomena must associate [20]. In theoretical calculations, we manage to match the physical systems of Avogadro's number of spins by setting the number of spins in the models to a mathematical infinity, $N \to \infty$. In traditional treatment, we often take this limit at the very beginning stage of calculations, which facilitates us to employ useful transforms, such as the substitution of the sum of momentum number q with an integral (in D dimensions), $(1/N)\sum_q[\cdots] = \int d^Dq/(2\pi)^D[\cdots]$, to work out desired quantities. Thus N will disappear in the final results. For example, critical spin chains have been found to exhibit algebraically decaying correlation functions [21,22] like

$$C_\infty(r) \sim \frac{b}{r^\eta}, \tag{1}$$

where b and η are real numbers and r is the distance between the two spins.

Can we defer the setting of the limit, $N \to \infty$, till the end of calculation? And if so, what can we get from it? In this work, we shall demonstrate that the concepts of locality and nonlocality can be well distinguished and defined for a ring system in the limit $N \to \infty$. We establish the full framework for extracting the nonlocal factors in the correlation function basing on an exactly solvable prototype—the transverse Ising ring at its phase transition point. Then we reappraise the usefulness of the finite-size scaling analysis in this framework and apply it to the isotropic XY and Heisenberg rings with emphasis on the effect of ring frustration. Note that in this paper we only consider the nonlocal behavior of correlation functions [23], which is quite different from the nonlocal behavior observed in the quantum measurements or quantum information.

We consider the spin correlation function of the ground state $|E_0\rangle$,

$$C^a_{r,N} = \langle E_0|\sigma^a_j\sigma^a_{j+r}|E_0\rangle, \tag{2}$$

where σ^a_j $(a = x, y, z)$ are Pauli matrices. Throughout the whole paper, we only consider the x component of the correlation function $C^x_{r,N}$. To ease the notation, we will drop the superscript and simply denote it as $C_{r,N}$.

Obviously, the correlations should satisfy the following cyclic relation (Fig. 1):

$$C_{r,N} = C_{N-r,N}. \tag{3}$$

The main idea is that the results may be different if the limit, $N \to \infty$, is made at two different occasions, as follows.

(i) If setting $N \to \infty$ at the beginning stage of calculation, we denote the resulting correlation function as $C_\infty(r)$. The example in Eq. (1) falls into this case.

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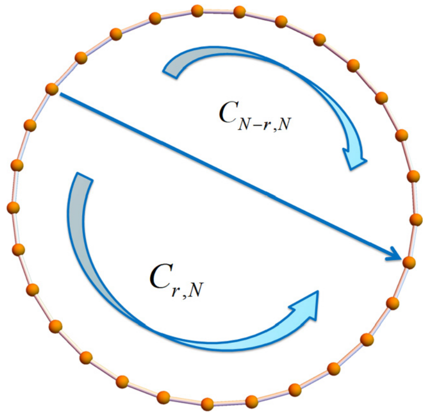

FIG. 1. Periodic spin chain. Ring frustration occurs if the number of spins is odd and the nearest-neighbor interactions are antiferromagnetic.

(ii) If setting $N \to \infty$ at the end of calculation, we get

$$C^{(O)}(r,\alpha) = \lim_{L\to\infty} C_{r,2L+1}, \tag{4}$$

$$C^{(E)}(r,\alpha) = \lim_{L\to\infty} C_{r,2L}, \tag{5}$$

for $N = 2L+1 \in$ Odd and $N = 2L \in$ Even, respectively, where we have defined a parameter

$$\alpha = \lim_{N\to\infty} \frac{r}{N}, \tag{6}$$

whose value can be restricted to the range $0 \leqslant \alpha < 1/2$ due to the ring geometry and the cyclic relation Eq. (3). The surprising difference between $C^{(O)}(r,\alpha)$ and $C^{(E)}(r,\alpha)$ will be exemplified.

It is natural to put the distances into three categories in the limit $N \to \infty$, as follows.

(i) The distance is *local* if $r \approx 1$.

(ii) The distance is *near local* if $r \gg 1$ and $\alpha = 0$, just like Eq. (1). Here the condition $r \gg 1$ is required to avoid the short-range and unstable behaviors.

(iii) The distance is *nonlocal* if $\alpha \neq 0$.

In this work, we shall first present a clear prototype, the transverse Ising ring at its phase transition point, to demonstrate the differences among $C_\infty(r)$, $C^{(O)}(r,\alpha)$, and $C^{(E)}(r,\alpha)$. More importantly, we propose three nonlocal factors defined as ratios. The first two of them are for the measure of nonlocality for $N = 2L+1 \in$ Odd and $N = 2L \in$ Even, respectively:

$$R^{(O)}(\alpha) = \frac{C^{(O)}(r,\alpha)}{C_\infty(r)}, \tag{7}$$

$$R^{(E)}(\alpha) = \frac{C^{(E)}(r,\alpha)}{C_\infty(r)}. \tag{8}$$

These definitions are possible only if the r dependence of the right hand sides of the above equations cancels out, as will be exemplified later. The third is for the measure of the effect of ring frustration,

$$R(\alpha) = \frac{R^{(O)}(\alpha)}{R^{(E)}(\alpha)}. \tag{9}$$

However, many models in the limit $N \to \infty$ cannot be solved as exactly as the transverse Ising ring at its phase transition point. So, instead of Eqs. (7)–(9), we have to conjecture the trends of the finite-size version of the ratios,

$$R^{(O)}_{r,2L+1} = \frac{C_{r,2L+1}}{C_\infty(r)} \longrightarrow R^{(O)}(\alpha), \tag{10}$$

$$R^{(E)}_{r,2L} = \frac{C_{r,2L}}{C_\infty(r)} \longrightarrow R^{(E)}(\alpha), \tag{11}$$

$$R_{r,2L+1} = \frac{R^{(O)}_{r,2L+1}}{R^{(E)}_{r,2L}} \longrightarrow R(\alpha), \tag{12}$$

with the system's size increasing. This is coincident with the famous finite-size scaling (FSS) hypothesis. In fact, as a scaling function, $R^{(E)}_{r,2L}$ has been studied tremendously by numerical methods for many models in the past decades [24], while the other two, $R^{(O)}_{r,2L+1}$ and $R_{r,2L+1}$, have been somewhat overlooked so far, till the effect of ring frustration makes them prominent [13]. And as one of the most important inferences, the scaling function observed in FSS analysis can truly approximate the nonlocal factor of an infinite system. This conclusion brings us an opportunity to utilize FSS as a valuable method for exploring the nonlocality in many-body systems. We address this by figuring out the nonlocal factors of the isotropic XY and spin-1/2 Heisenberg rings.

In the following, we present the analyses of three popular critical spin chains. As a prototype, the transverse Ising model at its transition point is exactly solved in Sec. II. The isotropic XY model is investigated numerically in Sec. III. In Sec. IV, the spin-1/2 Heisenberg model is investigated by the Bethe ansatz. At last, we give a conclusion.

II. CRITICAL TRANSVERSE ISING RING

In this section, we are concerned with a simple critical model, the transverse Ising model at its critical point (TIC),

$$H^{\mathrm{TIC}} = \sum_{j=1}^{N} \sigma_j^x \sigma_{j+1}^x - \sum_{j=1}^{N} \sigma_j^z, \tag{13}$$

which is a special case of the general XY Hamiltonian ($\gamma = 1, h = 1$),

$$H(\gamma,h) = \sum_{j=1}^{N} \left(\frac{1+\gamma}{2} \sigma_j^x \sigma_{j+1}^x + \frac{1-\gamma}{2} \sigma_j^y \sigma_{j+1}^y \right) - h \sum_{j=1}^{N} \sigma_j^z, \tag{14}$$

where γ and h are parameters for anisotropy and transverse field.

A. General formulas

For the general Hamiltonian, Eq. (14), we have the standard diagonalization procedure [25]. Here, we abbreviate the main formulas that will be used later. In the context of the so-called a-cycle problem of Jordan-Wigner fermions [26,27], we introduce the Jordan-Wigner transformation [28],

$$\sigma_j^+ = (\sigma_j^x + i\sigma_j^y)/2 = c_j^\dagger \exp\left(i\pi \sum_{l<j} c_l^\dagger c_l \right), \tag{15}$$

and Fourier transformation

$$c_q = \frac{1}{\sqrt{N}}\sum_{j=1}^{N} c_j \exp(iqj), \tag{16}$$

and diagonalize the fermionic Hamiltonian with Even(E) or Odd(O) number of lattice sites in the even(e) or odd(o) channels as (we use the same notations as those in Ref. [13])

$$H^{(E,o)} = \epsilon(0)(2c_0^\dagger c_0 - 1) + \epsilon(\pi)(2c_\pi^\dagger c_\pi - 1) + \sum_{q\in q^{(E,o)},q\neq 0,\pi} \omega(q)(2\eta_q^\dagger \eta_q - 1), \tag{17}$$

$$H^{(E,e)} = \sum_{q\in q^{(E,e)}} \omega(q)(2\eta_q^\dagger \eta_q - 1), \tag{18}$$

$$H^{(O,o)} = \epsilon(0)(2c_0^\dagger c_0 - 1) + \sum_{q\in q^{(O,o)},q\neq 0} \omega(q)(2\eta_q^\dagger \eta_q - 1), \tag{19}$$

$$H^{(O,e)} = \epsilon(\pi)(2c_\pi^\dagger c_\pi - 1) + \sum_{q\in q^{(O,e)},q\neq \pi} \omega(q)(2\eta_q^\dagger \eta_q - 1), \tag{20}$$

where

$$q^{(E,o)} = \left\{-\frac{N-2}{N}\pi, \ldots, -\frac{2}{N}\pi, 0, \frac{2}{N}\pi, \ldots, \frac{N-2}{N}\pi, \pi\right\}, \tag{21}$$

$$q^{(E,e)} = \left\{-\frac{N-1}{N}\pi, \ldots, -\frac{1}{N}\pi, \frac{1}{N}\pi, \ldots, \frac{N-1}{N}\pi\right\}, \tag{22}$$

$$q^{(O,e)} = \left\{-\frac{N-2}{N}\pi, \ldots, -\frac{1}{N}\pi, \frac{1}{N}\pi, \ldots, \frac{N-2}{N}\pi, \pi\right\}, \tag{23}$$

$$q^{(O,o)} = \left\{-\frac{N-1}{N}\pi, \ldots, -\frac{2}{N}\pi, 0, \frac{2}{N}\pi, \ldots, \frac{N-1}{N}\pi\right\}. \tag{24}$$

In the above, we have defined

$$\eta_q = u_q c_q - i v_q c_{-q}^\dagger \quad (q \neq 0, \pi), \tag{25}$$

with

$$u_q^2 = \frac{1}{2}\left(1 + \frac{\epsilon(q)}{\omega(q)}\right), \quad v_q^2 = \frac{1}{2}\left(1 - \frac{\epsilon(q)}{\omega(q)}\right),$$
$$2u_q v_q = \frac{\Delta(q)}{\omega(q)},$$
$$\epsilon(q) = \cos q - h, \quad \Delta(q) = \gamma \sin q,$$
$$\omega(q) = \sqrt{\epsilon(q)^2 + \Delta(q)^2}. \tag{26}$$

And in all of the four cases, fermion vacuums share the same form of BCS-type wave function,

$$|\phi^{(E/O,e/o)}\rangle = \prod_{q\,\in\, q^{(E/O,e/o)}\$0\,<\,q\,<\,\pi)} (u_q + i v_q c_q^\dagger c_{-q}^\dagger)|0\rangle, \tag{27}$$

above which quasiparticles are created. To restore the exact degrees of freedom of the original spin system, we erase the nonphysical states by projections. For $N = 2L \in$ Even, we use

$$H(\gamma, h) = P^+ H^{(E,e)} P^+ \oplus P^- H^{(E,o)} P^-, \tag{28}$$

and for $N = 2L + 1 \in$ Odd, we use

$$H(\gamma, h) = P^+ H^{(O,e)} P^+ \oplus P^- H^{(O,o)} P^-, \tag{29}$$

where the projectors $P^\pm = \frac{1}{2}[1 \pm \prod_{n=1}^{N}(1 - 2c_n^\dagger c_n)]$.

In such a tedious but faithful mapping, we clearly see the resemblance and difference between the spin Hamiltonian, Eq. (14), and the fermionic Hamiltonians, Eqs. (17)–(20). For bipartite lattice, i.e., $N = 2L \in$ Even, the ring frustration is absent, so the discrepancy is small and may be neglected. But when $N = 2L + 1 \in$ Odd, the system's bulk property is largely changed, because the ring frustration rumples the ground state and low-energy excited states [13,14].

B. Longitudinal correlation functions

1. $N = 2L \in Even$

The ground state is

$$\left|E_0^{(E,e)}\right\rangle = |\phi^{(E,e)}\rangle \tag{30}$$

and its energy reads

$$E_0^{(E,e)} = -\sum_{q\in q^{(E,e)}} \omega(q) \tag{31}$$

for all h including the critical point $h = 1$. The correlation function turns out to be a Toeplitz determinant that can be reduced to (Appendix A)

$$C_{r,N} = \left(-\frac{1}{N}\right)^r \det\left[\csc\frac{(\mu_j + \nu_k)\pi}{2N}\right]_{0\leqslant j,k\leqslant r-1}, \tag{32}$$

where

$$\mu_j = 2j + 1, \quad \nu_k = -2k. \tag{33}$$

Then, by making use of the identity (Appendix B),

$$\det\left[\frac{1}{\sin(a_i + b_j)}\right]_{0\leqslant i,j\leqslant n-1} = \frac{\prod_{0\leqslant i<j\leqslant n-1}\sin(a_i - a_j)\sin(b_i - b_j)}{\prod_{0\leqslant i,j\leqslant n-1}\sin(a_i + b_j)}, \tag{34}$$

we find an exact result (notice $N \in$ Even),

$$C_{r,N} = (-1)^r S_{r,N}, \tag{35}$$

where

$$S_{r,N} = \frac{\prod_{0\leqslant j<k\leqslant r-1}\sin\frac{(\mu_j-\mu_k)\pi}{2N}\sin\frac{(\nu_j-\nu_k)\pi}{2N}}{N^r\prod_{j=0}^{r-1}\prod_{k=0}^{r-1}\sin\frac{(\mu_j+\nu_k)\pi}{2N}}. \tag{36}$$

2. $N = 2L + 1 \in Odd$

The ground state is

$$\left|E_0^{(O,o)}\right\rangle = c_0^\dagger|\phi^{(O,o)}\rangle, \tag{37}$$

and its energy is

$$E_0^{(O,o)} = |1 - h| + (1 - h) - \sum_{q\in q^{(O,o)}} \omega(q) \tag{38}$$

for all h including the critical point $h = 1$. Its longitudinal correlation function is also represented by a Toeplitz determinant that can be reduced to (Appendix A)

$$C_{r,N} = \left(\frac{1}{N}\right)^r \det\left[1 - \cot\frac{(\mu_j + \nu_k)\pi}{2N}\right]_{0\leqslant j,k\leqslant r-1}. \quad (39)$$

And by making use of another identity (Appendix B),

$$\det\left[\frac{\cos(a_i + b_j + \phi)}{\sin(a_i + b_j)}\right]_{0\leqslant i,j\leqslant n-1} = \frac{\prod_{0\leqslant i<j\leqslant n-1}\sin(a_i - a_j)\sin(b_i - b_j)}{\prod_{0\leqslant i,j\leqslant n-1}\sin(a_i + b_j)} \times \cos\left[\sum_{i=0}^{n-1}(a_i + b_i) + \phi\right]\cos^{n-1}\phi, \quad (40)$$

we find another exact result (notice $N \in$ Odd),

$$C_{r,N} = (-1)^r B_1(\alpha) S_{r,N}, \quad (41)$$

where

$$B_1(\alpha) = \cos\frac{\alpha\pi}{2} - \sin\frac{\alpha\pi}{2}. \quad (42)$$

C. Nonlocal factors

It is helpful to review the traditional treatment at this moment. If we set $N \to \infty$, both Eqs. (35) and (41) will become the Cauchy determinant that leads to the well-known asymptotic formula [29–31],

$$C_\infty(r) \approx (-1)^r \frac{b_1}{r^{1/4}}, \quad (43)$$

where $b_1 = e^{1/4}2^{1/12}A^{-3} \approx 0.645002448$; A is the Glaisher's constant. However, this approximation obliterates the important difference between the systems with odd and even numbers of lattice sites N.

To get accurate results, let us focus on Eqs. (35) and (41). By denoting $\theta = \frac{\pi}{2N}$, we rewrite $S_{r,N}$ in Eq. (36) as

$$S_{r,N} = \frac{\prod_{1\leqslant m\leqslant r-1}(\cos^2\theta - \cot^2 m\theta\ \sin^2\theta)^{m-r}}{(N\ \sin\theta)^r}. \quad (44)$$

Then, noticing the identity (only exact for $N = 2L + 1$),

$$\frac{1}{N\ \sin\theta} = \prod_{1\leqslant m\leqslant L}(\cos^2\theta - \cot^2 m\theta\ \sin^2\theta), \quad (45)$$

we find that

$$\ln S_{r,N} = \sum_{m=1}^{r-1} m\ \ln(\cos^2\theta - \cot^2 m\theta\ \sin^2\theta) + r\sum_{m=r}^{L}\ln(\cos^2\theta - \cot^2 m\theta\ \sin^2\theta). \quad (46)$$

Next, by substituting the Taylor expansion,

$$\ln(\cos^2\theta - \cot^2 m\theta\ \sin^2\theta) = \ln\left(1 - \frac{1}{4m^2}\right) - \frac{1}{3}\theta^2 - \frac{1 + 24m^2}{90}\theta^4 - \cdots, \quad (47)$$

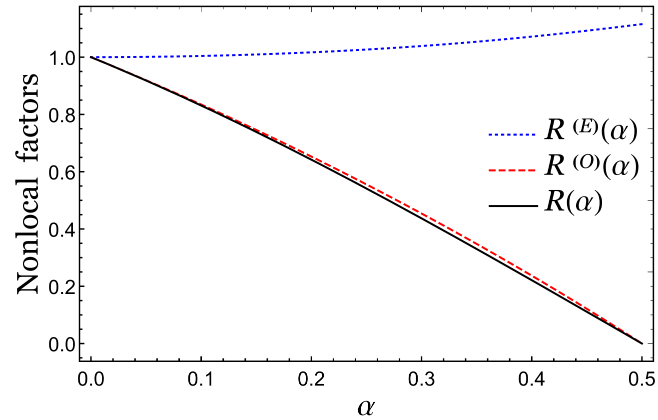

FIG. 2. Nonlocal factors of the transverse Ising ring at its phase transition point.

into Eq. (46) and accomplishing the summations with the index m, we arrive at

$$\ln S_{r,N} = -\frac{1}{4}\ln r + \ln b_1 + h(\alpha) + O\left(\frac{1}{N}\right), \quad (48)$$

where $h(\alpha)$ is a sum containing two convergent expansions (for more terms, please see Appendix C):

$$h(\alpha) = \frac{\alpha}{2} - \left(\frac{\pi^2\alpha^2}{24} + \frac{\pi^4\alpha^4}{240} + \cdots\right) - \left[\frac{\pi^2\alpha(1 - 2\alpha)}{24} + \frac{\pi^4\alpha(1 - 8\alpha^3)}{1440} + \cdots\right]. \quad (49)$$

At this last moment, we are able to keep the parameter $\alpha = \frac{r}{N}$ after ignoring the terms in order of $O(\frac{1}{N})$, and get

$$\lim_{N\to\infty} S_{r,N} = \frac{b_1}{r^{1/4}} e^{h(\alpha)}. \quad (50)$$

Now we can reap the accurate nonlocal factor,

$$R^{(O)}(\alpha) = e^{h(\alpha)} B_1(\alpha). \quad (51)$$

And it is easy to verify numerically that there holds an infinitesimal difference ($N = 2L + 1$),

$$S_{r,N} - S_{r,N-1} \sim \frac{1}{N^{5/4}} \to 0, \quad (52)$$

and the above calculation is also true for $N = 2L \to \infty$. Thus we get the other two nonlocal factors,

$$R^{(E)}(\alpha) = e^{h(\alpha)}, \quad (53)$$

$$R(\alpha) = B_1(\alpha). \quad (54)$$

The nonlocal factors are illustrated in Fig. 2. We see that $R^{(O)}(\alpha)$ and $R(\alpha)$ are quite close since $R^{(E)}(\alpha)$ deviates not far from 1.

III. ISOTROPIC *XY* RING

The isotropic XY model is given by

$$H^{XY} = \frac{1}{2}\sum_{j=1}^{N}\left(\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y\right), \quad (55)$$

which is also a special case of Eq. (14) as $H^{XY} = H(0, 0)$. In this model, we cannot compute its nonlocal factor analytically. However, its correlation functions can also be represented by Toeplitz determinant, which facilitates us to calculate systems as large as thousands of spins so that nonlocal factors can be deduced via convincing numerical evidence. The solution of its a-cycle problem is quite delicate [13,25,26]. It turns out that the systems with $N = 4K, 4K + 2 \in$ Even and $N = 4K + 1, 4K + 3 \in$ Odd should be solved separately (Appendix A). For simplicity and without loss of generality, we demonstrate the numerical results of $N = 4K \in$ Even and $N = 4K + 1 \in$ Odd here.

A. Nonlocal factor for $N = 4K \in$ Even

For $N = 4K \in$ Even the ground state is unique and the excitations are gapless. The correlation function is expressed by a Toeplitz determinant (Appendix A),

$$C_{r,N} = \det[\mathscr{T}_{j-k,N}]_{1\leqslant j,k\leqslant r}, \tag{56}$$

where the element reads

$$\mathscr{T}_{n,N} = \begin{cases} 0 & (n=1), \\ -\frac{2}{N}\csc\frac{\pi(n-1)}{N}\sin\frac{\pi(n-1)}{2} & (\text{other } n). \end{cases} \tag{57}$$

Again, at this moment, if setting the limit, $N \to \infty$, before the evaluation of the Toeplitz determinants, the element in Eq. (57) becomes the same one that was obtained originally by Lieb *et al.* [26],

$$\mathscr{T}_{n,\infty} \approx \begin{cases} 0 & (n \in \text{odd}), \\ \frac{2}{\pi(n-1)}\cos\frac{n\pi}{2} & (n \in \text{even}). \end{cases} \tag{58}$$

Basing on it, McCoy found an asymptotic formula [30],

$$C_\infty(r) \approx (-1)^r \frac{b_2}{r^{1/2}}, \tag{59}$$

where $b_2 = e^{1/2}2^{2/3}A^{-6} \approx 0.588\,352\,664$. It is easy to verify the original observation by Kaplan *et al.* that the numerical result of Eq. (56) deviates from Eq. (59) by a factor [24]

$$R^{(E)}(\alpha) = 1 + 0.28822\,\sinh^2(1.673\alpha). \tag{60}$$

This factor was ascribed to the finite-size effect. Now in the context of nonlocality, we can reasonably say it truly reflects the nonlocal property when the system's size approaches infinity.

B. Nonlocal factor for $N = 4K + 1 \in$ Odd and the effect of ring frustration

While for $N = 4K + 1 \in$ Odd, there are four degenerate ground states, without loss of generality, we deduce the correlation function for one of them as (Appendix A)

$$C_{r,N} = \det\left[\mathscr{T}_{j-k,N} + \frac{2\beta_{Q_o}}{N}e^{i(j-k)Q_o}\right]_{1\leqslant j,k\leqslant r}, \tag{61}$$

where $\beta_{Q_o} = \text{sgn}(\cos Q_o)e^{-iQ_o}$, $Q_o = \frac{N-1}{2N}\pi$, and

$$\mathscr{T}_{n,N} = \begin{cases} -\frac{1}{N} & (n=1), \\ -\frac{2}{N}\csc\frac{(n-1)\pi}{N}\sin\frac{(1+N)(n-1)\pi}{2N} & (\text{other } n). \end{cases} \tag{62}$$

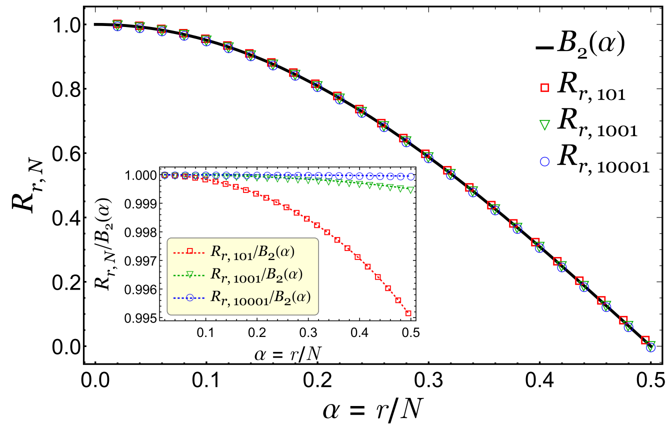

FIG. 3. $R_{r,N}$ with $N = 101,\ 1001$, and 10001 for the isotropic XY model. The data collapse to the proposed scaling curve $B_2(\alpha)$ very accurately. The ratios, $\frac{R_{r,N}}{B_2(\alpha)}$, in the inset demonstrate how the data approach the curve $B_2(\alpha)$ with N increasing.

We directly work out the data of $R_{r,N} = \frac{C_{r,N}}{C_{r,N-1}}$ with $N = 101, 1001, 10001$ according to Eq. (12). We found the data collapse to the curve,

$$B_2(\alpha) = \left(\cos\frac{\alpha\pi}{2}\right)^2 - \left(\sin\frac{\alpha\pi}{2}\right)^2, \tag{63}$$

very accurately (Fig. 3), which suggests the nonlocal factor due to pure ring frustration is

$$R(\alpha) = \lim_{N\to\infty} R_{r,N} = B_2(\alpha). \tag{64}$$

The nonlocal factor $R^{(O)}(\alpha)$ can be inferred from Eqs. (60) and (64) easily.

IV. SPIN-1/2 HEISENBERG CHAIN WITH RING FRUSTRATION

In this section, we turn to the isotropic spin-1/2 Heisenberg model with ring frustration. The Hamiltonian is

$$H^H = J\sum_{i=1}^{N}\left(S_i^xS_{i+1}^x + S_i^yS_{i+1}^y + S_i^zS_{i+1}^z\right). \tag{65}$$

Similar to the XY model, here we impose the periodic boundary condition $S_{N+1}^a = S_1^a$ for $a = x, y, z$ and only consider the antiferromagnetic interacting $J > 0$ with odd number of sites.

It is well known that the Heisenberg model can be exactly solved by the Bethe ansatz. Here we only present the results we need for the calculations of ground state correlation functions; detailed derivation can be found in [22,32]. First the number of down spins $N_\downarrow$ is conserved in the Heisenberg model; thus we can diagonalize the Hamiltonian in each sub-Hilbert space with fixed number of down spins. Since $J > 0$ and N is odd, the ground states occur in the subspace with $N_\downarrow = (N-1)/2$ or $N_\downarrow = (N+1)/2$. These two subspaces can be mapped to each other by a spin flip of all spins. Therefore, we only need to consider the case with $N_\downarrow = (N-1)/2$.

The eigenfunction can be expressed as

$$|\psi\rangle = \sum_{n_1,\ldots,n_{N_\downarrow}} f(n_1, n_2, \ldots, n_{N_\downarrow})|n_1, n_2, \ldots, n_{N_\downarrow}\rangle. \quad (66)$$

Here $|n_1, n_2, \ldots, n_{N_\downarrow}\rangle$ denotes the spin state with $N_\downarrow$ down spins located at lattice site n_1 to $n_{N_\downarrow}$, while all other sites are spin up.

The ground state wave function $f(n_1, \ldots, n_M)$ can be obtained by the exact solution of Bethe ansatz or direct numerical digonalization. Because the computation complexity increases exponentially with the number of spins, in both cases, one can only compute the ground state wave function with the number of spins up to around $N = 30$. For our demonstration purpose, we have only computed the ground state and correlations $C_{r,N}$ for lattices with number of spins from $N = 10$ to 21. The method of Bethe ansatz for odd number of spins is briefly reviewed in Appendix D.

Once the ground state wave function is obtained, the ground state correlation is given by

$$C_{r,N} = \langle S_1^z S_r^z \rangle = \frac{\sum \prod_{j=1}^{N_\downarrow} (-1)^{\delta_{n_j 1}} (-1)^{\delta_{n_j r}} |f(n_1,\ldots,n_{N_\downarrow})|^2}{4 \sum |f(n_1,\ldots,n_{N_\downarrow})|^2}. \quad (67)$$

For a periodic chain with even number of lattice sites, the asymptotic formula of correlation function is

$$C_\infty(r) = b(-1)^r \frac{\sqrt{\ln r}}{r}, \quad (68)$$

with $b \approx 0.56$. The nonlocal factors have been obtained in [33] as follows:

$$R^{(E)}(\alpha) = [1 + 0.288\,22\,\sinh^2(1.673\alpha)]^{1.805}, \quad (69)$$

which fits well our data for an even number of lattice sites. To see clearly the effect of ring frustration due to the odd number of lattice sites, we directly produce new sequences of data from the ones by the Bethe ansatz according to

$$R_{r,N} = \frac{C_{r,N}}{C_{r,N-1}}. \quad (70)$$

The result is shown in Fig. 4. We see the data also collapse to the curve $B_2(\alpha)$ quite well although our data are too few

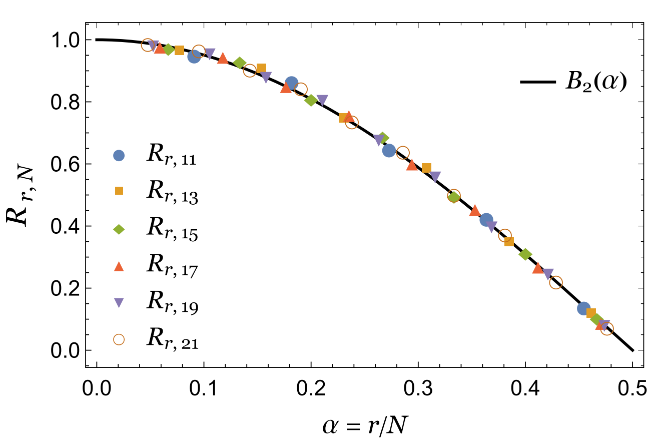

FIG. 4. $R_{r,N}$ with N from 11 to 21 for the spin-1/2 Heisenberg model. The data collapse to the proposed scaling curve $B_2(\alpha)$ very well.

($N = 11$ to 21), which suggests that $B_2(\alpha)$ is the true nonlocal factor $R(\alpha)$ in the thermodynamic limit.

V. CONCLUSION

In this paper, we propose a well-defined concept of nonlocality in the infinite spin rings. Three popular critical spin models are presented as cases in point. The transverse Ising ring serves as a prototype since it is exactly solvable. Basing on it, we establish the framework for extracting the nonlocal factors in the correlation functions with emphasis on the effect of ring frustration. The usefulness of FSS analysis is demonstrated by numerical solutions of the nonlocal factors in the correlation functions of isotropic XY and spin-1/2 Heisenberg rings.

In brief, both $C^{(E)}(r, \alpha)$ and $C^{(O)}(r, \alpha)$ of the three typical critical models considered in this work are factorizable in the limit $N \to \infty$,

$$C^{(E)}(r, \alpha) = R^{(E)}(\alpha) C_\infty(r), \quad (71)$$

$$C^{(O)}(r, \alpha) = R^{(O)}(\alpha) C_\infty(r) = R(\alpha) R^{(E)}(\alpha) C_\infty(r), \quad (72)$$

which demonstrate clearly that $N \in \text{Even} \to \infty$ and $N \in \text{Odd} \to \infty$ render different nonlocal factors $R^{(E)}(\alpha)$ and $R^{(O)}(\alpha)$, respectively. Furthermore, $R^{(E)}(\alpha)$ and $R(\alpha)$ are responsible for the quantum frustration [2,4–7] and pure geometrical frustration, respectively.

The observed algebraically decaying $C_\infty(r)$ is a standard outcome of the continuous conformal field theories [22]. Through FSS analysis, $R^{(E)}(\alpha)$ has been revealed in many works [24,33]. The effects of odd number of spins have also been considered by many authors previously. For example, the ground state energy and short-ranged correlations of the XXZ model with odd number of spins were computed in [34]. The scaling properties of ground state energy and zero-temperature susceptibility of the same model are also studied in [35]. The long-range correlation function for the antiferromagnetic (*noncritical*) phase of the transverse Ising chain with ring frustration were studied in [11,13,14], which present a consistent nonlocal factor, $R(\alpha) = 1 - 2\alpha$. Now we can also think that the model in the same parameter region exhibits the other two trivial nonlocal factors, $R^{(E)}(\alpha) = 1$ and $R^{(O)}(\alpha) = R(\alpha)$. To capture the physical effects of odd number of spins in a continuum field theory model, one possible approach is to introduce a generalized boundary condition in a free fermion model. It may generate the kink states [13] appearing in the antiferromagnetic phase of the transverse Ising chain. However, how to quantitatively account for all the nonlocal factors by a continuum field theory is still unknown. We may explore these questions in the future.

ACKNOWLEDGMENTS

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APPENDIX A: TOEPLITZ DETERMINANT REPRESENTATION FOR THE CORRELATION FUNCTIONS

1. Transverse Ising ring at its critical point

The transverse Ising model at its critical point reads ($\gamma = 1, h = 1$)

$$H(1,1) = H^{\mathrm{TIC}} = \sum_{j=1}^{N} \sigma_j^x \sigma_{j+1}^x - \sum_{j=1}^{N} \sigma_j^z. \tag{A1}$$

a. $N = 2L \in Even$

When $N = 2L \in$ Even, the ground state is

$$\left|E_0^{(E,e)}\right\rangle = |\phi^{(E,e)}\rangle \tag{A2}$$

and its energy reads

$$E_0^{(E,e)} = -\sum_{q\in q^{(E,e)}} \omega(q), \tag{A3}$$

according to Eq. (28). By introducing the notations $A_j = c_j^\dagger + c_j$ and $B_j = c_j^\dagger - c_j$, applying the Wick's theorem in respect of $|\phi^{(E,e)}\rangle$, and retaining the nonzero contractions, $\langle\phi^{(E,e)}|B_l A_m|\phi^{(E,e)}\rangle = \mathscr{D}_{l-m+1}^{(E,e)}$, the longitudinal correlation function is rewritten in a Toeplitz determinant,

$$C_{r,N} = \langle\phi^{(E,e)}|B_j A_{j+1} \dots B_{j+r-1} A_{j+r}|\phi^{(E,e)}\rangle = \begin{vmatrix} \mathscr{D}_0^{(E,e)} & \mathscr{D}_{-1}^{(E,e)} & \dots & \mathscr{D}_{-r+1}^{(E,e)} \\ \mathscr{D}_1^{(E,e)} & \mathscr{D}_0^{(E,e)} & \dots & \mathscr{D}_{-r+2}^{(E,e)} \\ \dots & \dots & \dots & \dots \\ \mathscr{D}_{r-1}^{(E,e)} & \mathscr{D}_{r-2}^{(E,e)} & \dots & \mathscr{D}_0^{(E,e)} \end{vmatrix}, \tag{A4}$$

where

$$\mathscr{D}_n^{(E,e)} = \frac{1}{N} \sum_{q\in q^{(E,e)}} D(e^{iq}) e^{-iqn}, \tag{A5}$$

$$D(e^{iq}) = e^{iq}\left(1 - 2u_q^2 + 2iu_q v_q\right). \tag{A6}$$

Since (due to $\gamma = 1, h = 1$)

$$D(e^{iq}) = i\ \mathrm{sgn}(q) e^{iq/2}, \tag{A7}$$

we have

$$\mathscr{D}_r^{(E,e)} = -\frac{1}{N} \csc\frac{(1-2r)\pi}{2N}. \tag{A8}$$

Thus, for $N = 2L \in$ Even, we get the abbreviated correlation function in the paper [Eq. (32)],

$$C_{r,N} = \left(-\frac{1}{N}\right)^r \det\left[\csc\frac{(\mu_j + \nu_k)\pi}{2N}\right]_{1\leqslant j,k\leqslant r}, \tag{A9}$$

where $\mu_j = 2j + 1$ and $\nu_k = -2k$.

b. $N = 2L + 1 \in Odd$

When $N = 2L + 1 \in$ Odd, the ground state is

$$\left|E_0^{(O,o)}\right\rangle = c_0^\dagger|\phi^{(O,o)}\rangle \tag{A10}$$

and its energy is

$$E_0^{(O,o)} = -\sum_{q\in q^{(O,o)}} \omega(q), \tag{A11}$$

according to Eq. (29). For the ground state $|E_0^{(O,o)}\rangle$, we need to apply the Wick's theorem in respect of $|\phi^{(O,o)}\rangle$,

$$C_{r,N} = \langle\phi^{(O,o)}|c_0 B_j A_{j+1} \dots B_{j+r-1} A_{j+r} c_0^\dagger|\phi^{(O,o)}\rangle. \tag{A12}$$

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

$$\begin{aligned} C_{r,N} &= \langle\phi^{(O,o)}|B_j A_{j+1} \dots B_{j+r-1} A_{j+r}|\phi^{(O,o)}\rangle \\ &\quad + \frac{2}{N}\langle\phi^{(O,o)}|B_{j+1} A_{j+2} \dots B_{j+r-1} A_{j+r}|\phi^{(O,o)}\rangle \\ &\quad + \frac{2}{N}\langle\phi^{(O,o)}|A_{j+1} B_{j+1} B_{j+2} A_{j+3} \dots B_{j+r-1} A_{j+r}|\phi^{(O,o)}\rangle \\ &\quad + \cdots. \end{aligned} \tag{A13}$$

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

$$\mathscr{D}_n^{(O,o)} = -\frac{1}{N} + \frac{1}{N} \sum_{q\,\in\, q^{(O,o)},\, q\neq 0} D(e^{iq}) e^{-iqn}, \tag{A14}$$

we can deduce the result as

$$C_{r,N} = \begin{vmatrix} \mathscr{D}_0^{(O,o)} & \mathscr{D}_{-1}^{(O,o)} & \dots & \mathscr{D}_{1-r}^{(O,o)} \\ \mathscr{D}_1^{(O,o)} & \mathscr{D}_0^{(O,o)} & \dots & \mathscr{D}_{2-r}^{(O,o)} \\ \dots & \dots & \dots & \dots \\ \mathscr{D}_{r-1}^{(O,o)} & \mathscr{D}_{r-2}^{(O,o)} & \dots & \mathscr{D}_0^{(O,o)} \end{vmatrix} + \begin{vmatrix} \frac{2}{N} & \frac{2}{N} & \dots & \frac{2}{N} \\ \mathscr{D}_1^{(O,o)} & \mathscr{D}_0^{(O,o)} & \dots & \mathscr{D}_{2-r}^{(O,o)} \\ \dots & \dots & \dots & \dots \\ \mathscr{D}_{r-1}^{(O,o)} & \mathscr{D}_{r-2}^{(O,o)} & \dots & \mathscr{D}_0^{(O,o)} \end{vmatrix} + \cdots + \begin{vmatrix} \mathscr{D}_0^{(O,o)} & \mathscr{D}_{-1}^{(O,o)} & \dots & \mathscr{D}_{1-r}^{(O,o)} \\ \mathscr{D}_1^{(O,o)} & \mathscr{D}_0^{(O,o)} & \dots & \mathscr{D}_{2-r}^{(O,o)} \\ \dots & \dots & \dots & \dots \\ \frac{2}{N} & \frac{2}{N} & \dots & \frac{2}{N} \end{vmatrix}$$

$$= \begin{vmatrix} \mathscr{D}_0^{(O,o)} + \frac{2}{N} & \mathscr{D}_{-1}^{(O,o)} + \frac{2}{N} & \dots & \mathscr{D}_{1-r}^{(O,o)} + \frac{2}{N} \\ \mathscr{D}_1^{(O,o)} + \frac{2}{N} & \mathscr{D}_0^{(O,o)} + \frac{2}{N} & \dots & \mathscr{D}_{2-r}^{(O,o)} + \frac{2}{N} \\ \vdots & \vdots & \vdots & \vdots \\ \mathscr{D}_{r-1}^{(O,o)} + \frac{2}{N} & \mathscr{D}_{r-2}^{(O,o)} + \frac{2}{N} & \dots & \mathscr{D}_0^{(O,o)} + \frac{2}{N} \end{vmatrix}. \tag{A15}$$

And since (due to $\gamma = 1, h = 1$)

$$D(e^{iq}) = i\ \mathrm{sgn}(q)e^{iq/2}, \tag{A16}$$

we have

$$\mathscr{D}_r^{(O,o)} = -\frac{1}{N} - \frac{1}{N}\cot\frac{(1-2r)\pi}{2N}. \tag{A17}$$

Thus for $N = 2L+1 \in$ Odd, we get the Toeplitz determinant representation of the correlation function in the paper [Eq. (39)]

$$C_{r,N} = \left(\frac{1}{N}\right)^r \det\left[1 - \cot\frac{(\mu_j+\nu_k)\pi}{2N}\right]_{0\leqslant j,k\leqslant r-1}. \tag{A18}$$

2. Isotropic XY ring

The isotropic XY model reads ($\gamma = 0, h = 0$)

$$H(0,0) = H^{XY} = \frac{1}{2}\sum_{j=1}^{N}\left(\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y\right). \tag{A19}$$

The situation in the XY ring is more delicate than that in the transverse Ising ring. The solutions for the ground state ought to be put into four categories, as follows.

(a) For $N = 4K$ ($K = 1, 2, 3, \ldots$), the ground state is unique, which reads $|\phi^{(E,e)}\rangle$.

(b) For $N = 4K+2$, the ground state is unique, which reads $c_\pi^\dagger|\phi^{(E,o)}\rangle$.

(c) For $N = 4K+1$, the ground states are fourfold degenerate due to the presence of ring frustration. Two of them come from the odd channel,

$$\left|E_{\pm Q_o}^{(O,o)}\right\rangle = \eta_{\pm Q_o}^\dagger|\phi^{(O,o)}\rangle, \tag{A20}$$

and two of them from the even channel,

$$\left|E_{\pm Q_e}^{(O,e)}\right\rangle = \eta_{\pm Q_e}^\dagger c_\pi^\dagger|\phi^{(O,e)}\rangle, \tag{A21}$$

where the characteristic wave vectors are

$$Q_o = \frac{N-1}{2N}\pi, \quad Q_e = \frac{N+1}{2N}\pi. \tag{A22}$$

(d) For $N = 4K+3$, the ground states are fourfold degenerate due to the presence of ring frustration. They are also expressed by Eqs. (A20) and (A21), but the characteristic wave vector swaps

$$Q_o = \frac{N+1}{2N}\pi, \quad Q_e = \frac{N-1}{2N}\pi. \tag{A23}$$

Let us demonstrate their correlation functions in Toeplitz determinant representation one by one.

a. $N = 4K \in Even$

In this case, because the ground state is $|\phi^{(E,e)}\rangle$, the correlation function shares the same expressions as that in Eqs. (A4)–(A6), but the elements are different and read

$$\mathscr{D}_r^{(E,e)} = \begin{cases} 0 & (r=1), \\ -\frac{2}{N}\csc\frac{\pi(r-1)}{N}\sin\frac{\pi(r-1)}{2} & (\text{other } r), \end{cases} \tag{A24}$$

since now we have

$$D(e^{iq}) = -\,\mathrm{sgn}(\cos q)e^{iq}. \tag{A25}$$

b. $N = 4K+2 \in Even$

In this case, the ground state is $c_\pi^\dagger|\phi^{(E,o)}\rangle$. We need to apply the Wick's theorem in respect of $|\phi^{(E,o)}\rangle$,

$$C_{r,N} = \langle\phi^{(E,o)}|c_\pi B_jA_{j+1}\ldots B_{j+r-1}A_{j+r}c_\pi^\dagger|\phi^{(E,o)}\rangle. \tag{A26}$$

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

$$\begin{aligned} C_{r,N} = {} & \langle\phi^{(E,o)}|B_jA_{j+1}\ldots B_{j+r-1}A_{j+r}|\phi^{(E,o)}\rangle - \frac{2}{N}\langle\phi^{(E,o)}|B_{j+1}A_{j+2}\ldots B_{j+r-1}A_{j+r}|\phi^{(E,o)}\rangle \\ & - \frac{2}{N}\langle\phi^{(E,o)}|A_{j+1}B_{j+1}B_{j+2}A_{j+3}\ldots B_{j+r-1}A_{j+r}|\phi^{(E,o)}\rangle + \cdots. \end{aligned} \tag{A27}$$

Then, by nonzero contractions, $\langle\phi^{(E,o)}|B_lA_m|\phi^{(E,o)}\rangle = \mathscr{D}_{l-m+1}^{(E,o)}$, with

$$\mathscr{D}_n^{(E,o)} = -\frac{1}{N} + \frac{1}{N}\sum_{q\,\in\, q^{(E,o)},\, q\neq\pi} D(e^{iq})e^{-iqn}, \tag{A28}$$

$$D(e^{iq}) = e^{iq}\left(1 - 2u_q^2 + 2iu_qv_q\right), \tag{A29}$$

we get

$$C_{r,N} = \begin{vmatrix} \mathscr{D}_0^{(E,o)} - \frac{2}{N} & \mathscr{D}_{-1}^{(E,o)} - \frac{2}{N}e^{-i\pi} & \cdots & \mathscr{D}_{-(r-1)}^{(E,o)} - \frac{2}{N}e^{-i(r-1)\pi} \\ \mathscr{D}_1^{(E,o)} - \frac{2}{N}e^{i\pi} & \mathscr{D}_0^{(E,o)} - \frac{2}{N} & \cdots & \mathscr{D}_{-(r-2)}^{(E,o)} - \frac{2}{N}e^{-i(r-2)\pi} \\ \vdots & \vdots & \vdots & \vdots \\ \mathscr{D}_{r-1}^{(E,o)} - \frac{2}{N}e^{i(r-1)\pi} & \mathscr{D}_{r-2}^{(E,o)} - \frac{2}{N}e^{-i(r-2)\pi} & \cdots & \mathscr{D}_0^{(E,o)} - \frac{2}{N} \end{vmatrix}. \tag{A30}$$

For the isotropic XY model ($\gamma = 0, h = 0$), we have

$$D(e^{iq}) = -\operatorname{sgn}(\cos q)e^{iq}, \tag{A31}$$

so we get

$$\mathscr{D}_n^{(E,o)} = \begin{cases} -\frac{2}{N} & (n=1), \\ -\frac{2}{N} - \frac{4}{N}\csc\frac{\pi(n-1)}{N}\sin\frac{\pi(n-1)}{2}\big[\sin\frac{(N-2)(n-1)\pi}{4N}\big]^2 & (\text{other } n). \end{cases} \tag{A32}$$

c. $N = 4K + 1 \in$ *Odd*

The ground states are of four degeneracy. For simplicity and without loss of generality, let us choose the state $|E_{Q_o}^{(O,o)}\rangle = \eta_{Q_o}^\dagger|\phi^{(O,o)}\rangle$. The starting point is

$$C_{r,N} = \langle\phi^{(O,o)}|\eta_{Q_o}B_jA_{j+1}\dots B_{j+r-1}A_{j+r}\eta_{Q_o}^\dagger|\phi^{(O,o)}\rangle. \tag{A33}$$

Likewise, the strategy is to eliminate the operators η_{Q_o} and $\eta_{Q_o}^\dagger$ first. Except for $\langle\phi^{(O,o)}|\eta_{Q_o}\eta_{Q_o}^\dagger|\phi^{(O,o)}\rangle = 1$, we find the combined nonzero contractions are very useful

$$\langle\phi^{(O,o)}|\eta_{Q_o}B_l|\phi^{(O,o)}\rangle\langle\phi^{(O,o)}|A_m\eta_{Q_o}^\dagger|\phi^{(O,o)}\rangle = \frac{\beta_{Q_o}}{N}e^{iQ_o(l-m+1)}, \tag{A34}$$

$$\beta_{Q_o} = -D(e^{-iQ_o}), \tag{A35}$$

so we could write down

$$\begin{aligned} 2C_{r,N} = &\bigg[\langle\phi^{(O,o)}|B_jA_{j+1}\dots B_{j+r-1}A_{j+r}|\phi^{(O,o)}\rangle + \frac{2\beta_{Q_o}}{N}\langle\phi^{(O,o)}|B_{j+1}A_{j+2}\dots B_{j+r-1}A_{j+r}|\phi^{(O,o)}\rangle \\ &+ \frac{2\beta_{Q_o}e^{-iQ_o}}{N}\langle\phi^{(O,o)}|A_{j+1}B_{j+1}B_{j+2}A_{j+3}\dots B_{j+r-1}A_{j+r}|\phi^{(O,o)}\rangle + \cdots\bigg] \\ &+ \bigg[\langle\phi^{(O,o)}|B_jA_{j+1}\dots B_{j+r-1}A_{j+r}|\phi^{(O,o)}\rangle + \frac{2\beta_{-Q_o}}{N}\langle\phi^{(O,o)}|B_{j+1}A_{j+2}\dots B_{j+r-1}A_{j+r}|\phi^{(O,o)}\rangle \\ &+ \frac{2\beta_{-Q_o}e^{iQ_o}}{N}\langle\phi^{(O,o)}|A_{j+1}B_{j+1}B_{j+2}A_{j+3}\dots B_{j+r-1}A_{j+r}|\phi^{(O,o)}\rangle + \cdots\bigg]. \end{aligned} \tag{A36}$$

The terms are grouped into two square brackets. Thus the correlation function can be represented by the sum of two Toeplitz determinants,

$$C_{r,N} = \tfrac{1}{2}\big[\Gamma^{(O,o)}\big(r, N, \beta_{Q_o}, e^{iQ_o}\big) + \Gamma^{(O,o)}\big(r, N, \beta_{-Q_o}, e^{-iQ_o}\big)\big] = \mathrm{Re}\big[\Gamma^{(O,o)}\big(r, N, \beta_{Q_o}, e^{iQ_o}\big)\big], \tag{A37}$$

where Re[ ] means taking the real part of the number and the determinant $\Gamma^{(O,o)}(r, N, \beta_{Q_o}, e^{iQ_o})$ reads

$$\Gamma^{(O,o)}(r, N, \beta_{Q_o}, e^{iQ_o}) = \begin{vmatrix} \mathscr{D}_0^{(O,o)} + \frac{2\beta_{Q_o}}{N} & \mathscr{D}_{-1}^{(O,o)} + \frac{2\beta_{Q_o}}{N}e^{-iQ_o} & \cdots & \mathscr{D}_{1-r}^{(O,o)} + \frac{2\beta_{Q_o}}{N}e^{i(1-r)Q_o} \\ \mathscr{D}_1^{(O,o)} + \frac{2\beta_{Q_o}}{N}e^{iQ_o} & \mathscr{D}_0^{(O,o)} + \frac{2\beta_{Q_o}}{N} & \cdots & \mathscr{D}_{2-r}^{(O,o)} + \frac{2\beta_{Q_o}}{N}e^{i(2-r)Q_o} \\ \vdots & \vdots & \vdots & \vdots \\ \mathscr{D}_{r-1}^{(O,o)} + \frac{2\beta_{Q_o}}{N}e^{i(r-1)Q_o} & \mathscr{D}_{r-2}^{(O,o)} + \frac{2\beta_{Q_o}}{N}e^{i(r-2)Q_o} & \cdots & \mathscr{D}_0^{(O,o)} + \frac{2\beta_{Q_o}}{N} \end{vmatrix}, \tag{A38}$$

with

$$\beta_{Q_o} = -D(e^{-iQ_o}) = \operatorname{sgn}(\cos Q_o)e^{-iQ_o}. \tag{A39}$$

$\mathscr{D}_n^{(O,o)}$ is defined in Eq. (A14) and we have

$$\mathscr{D}_n^{(O,o)} = \begin{cases} -\frac{1}{N} & (n=1), \\ -\frac{2}{N}\csc\frac{(n-1)\pi}{N}\sin\frac{(N+1)(n-1)\pi}{2N} & (\text{other } n). \end{cases} \tag{A40}$$

d. $N = 4K + 3 \in Odd$

We also choose the state $|E_{Q_o}^{(O,o)}\rangle = \eta_{Q_o}^{\dagger}|\phi^{(O,o)}\rangle$. It turns out the deduction is almost the same as that for $N = 4K + 1$, except for the final expression for $\mathscr{D}_n^{(O,o)}$,

$$\mathscr{D}_n^{(O,o)} = \begin{cases} \frac{1}{N} & (n = 1), \\ -\frac{2}{N} \csc \frac{(n-1)\pi}{N} \sin \frac{(N-1)(n-1)\pi}{2N} & (\text{other } n). \end{cases} \tag{A41}$$

APPENDIX B: DERIVATION OF EQS. (34) AND (40)

We will first prove the identity Eq. (40) by mathematical recursion. For convenience, we repeat Eq. (40) here:

$$D_n(\phi) = \det\left[\frac{\cos(a_i + b_j + \phi)}{\sin(a_i + b_j)}\right]_{1\leqslant i,j\leqslant n} = \frac{\prod_{1\leqslant i<j\leqslant n}\sin(a_i - a_j)\sin(b_i - b_j)}{\prod_{1\leqslant i,j\leqslant n}\sin(a_i + b_j)}\cos\left[\sum_{i=1}^{n}(a_i + b_i) + \phi\right]\cos^{n-1}\phi. \tag{B1}$$

Write out $D_n(\phi)$ explicitly as

$$D_n(\phi) = \begin{vmatrix} \frac{\cos(a_1+b_1+\phi)}{\sin(a_1+b_1)} & \frac{\cos(a_1+b_2+\phi)}{\sin(a_1+b_2)} & \cdots & \frac{\cos(a_1+b_n+\phi)}{\sin(a_1+b_n)} \\ \frac{\cos(a_2+b_1+\phi)}{\sin(a_2+b_1)} & \frac{\cos(a_2+b_2+\phi)}{\sin(a_2+b_2)} & \cdots & \frac{\cos(a_2+b_n+\phi)}{\sin(a_2+b_n)} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\cos(a_n+b_1+\phi)}{\sin(a_n+b_1)} & \frac{\cos(a_n+b_2+\phi)}{\sin(a_n+b_2)} & \cdots & \frac{\cos(a_n+b_n+\phi)}{\sin(a_n+b_n)} \end{vmatrix}. \tag{B2}$$

Subtracting the last column from all previous columns, we find

$$D_n(\phi) = \begin{vmatrix} \frac{-\cos\phi\,\sin(b_1-b_n)}{\sin(a_1+b_1)\sin(a_1+b_n)} & \frac{-\cos\phi\,\sin(b_2-b_n)}{\sin(a_1+b_2)\sin(a_1+b_n)} & \cdots & \frac{\cos(a_1+b_n+\phi)}{\sin(a_1+b_n)} \\ \frac{-\cos\phi\,\sin(b_1-b_n)}{\sin(a_2+b_1)\sin(a_2+b_n)} & \frac{-\cos\phi\,\sin(b_1-b_n)}{\sin(a_2+b_2)\sin(a_2+b_n)} & \cdots & \frac{\cos(a_2+b_n+\phi)}{\sin(a_2+b_n)} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{-\cos\phi\,\sin(b_1-b_n)}{\sin(a_n+b_1)\sin(a_n+b_n)} & \frac{-\cos\phi\,\sin(b_2-b_n)}{\sin(a_n+b_2)\sin(a_n+b_n)} & \cdots & \frac{\cos(a_n+b_n+\phi)}{\sin(a_n+b_n)} \end{vmatrix}$$

$$= (-\cos\phi)^{n-1}\frac{\prod_{i=1}^{n-1}\sin(b_i - b_n)}{\prod_{j=1}^{n}\sin(a_j + b_n)}\begin{vmatrix} \frac{1}{\sin(a_1+b_1)} & \frac{1}{\sin(a_1+b_2)} & \cdots & \cos(a_1+b_n+\phi) \\ \frac{1}{\sin(a_2+b_1)} & \frac{1}{\sin(a_2+b_2)} & \cdots & \cos(a_2+b_n+\phi) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{\sin(a_n+b_1)} & \frac{1}{\sin(a_n+b_2)} & \cdots & \cos(a_n+b_n+\phi) \end{vmatrix}. \tag{B3}$$

In the above determinant, multiply the last row by $\frac{-\cos(a_i+b_n+\phi)}{\cos(a_n+b_n+\phi)}$ and add to the ith row for $i = 1, \ldots, n-1$. For the element at (i, j), we have

$$\frac{1}{\sin(a_i + b_j)} + \frac{1}{\sin(a_n + b_j)}\frac{-\cos(a_i + b_n + \phi)}{\cos(a_n + b_n + \phi)} = \frac{-\cos(a_i + b_j + a_n + b_n + \phi)\sin(a_i - a_n)}{\sin(a_i + b_j)\sin(a_n + b_j)\cos(a_n + b_n + \phi)}. \tag{B4}$$

Making use of this identity, extracting the common factor for each row and column, and defining $\phi' = \phi + a_n + b_n$, we find

$$D_n(\phi) = \left(\frac{\cos\phi}{\cos\phi'}\right)^{n-1}\frac{\prod_{i=1}^{n-1}\sin(b_i - b_n)\sin(a_i - a_n)}{\prod_{j=1}^{n}\sin(a_j + b_n)\prod_{j=1}^{n-1}\sin(a_n + b_j)}\begin{vmatrix} \frac{\cos(a_1+b_1+\phi')}{\sin(a_1+b_1)} & \frac{\cos(a_1+b_2+\phi')}{\sin(a_1+b_2)} & \cdots & 0 \\ \frac{\cos(a_2+b_1+\phi')}{\sin(a_2+b_1)} & \frac{\cos(a_2+b_2+\phi')}{\sin(a_2+b_2)} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & \cos\phi' \end{vmatrix}$$

$$= \frac{\cos^{n-1}\phi}{\cos^{n-2}\phi'}\frac{\prod_{i=1}^{n-1}\sin(b_i - b_n)\sin(a_i - a_n)}{\prod_{j=1}^{n}\sin(a_j + b_n)\prod_{j=1}^{n-1}\sin(a_n + b_j)}D_{n-1}(\phi'). \tag{B5}$$

By mathematical recursion assumption, we have

$$D_{n-1}(\phi') = \frac{\prod_{1\leqslant i<j\leqslant n-1}\sin(a_i - a_j)\sin(b_i - b_j)}{\prod_{1\leqslant i,j\leqslant n-1}\sin(a_i + b_j)}\cos\left[\sum_{i=1}^{n-1}(a_i + b_i) + \phi'\right]\cos^{n-1}\phi'. \tag{B6}$$

Plugging Eq. (B6) into Eq. (B5), we get back Eq. (B1), which finishes the proof of Eq. (40).

We then prove the identity Eq. (34) again by mathematical recursion. For convenience, we repeat Eq. (34) here:

$$A_n = \det\left[\frac{1}{\sin(a_i+b_j)}\right]_{1\leqslant i,j\leqslant n} = \frac{\prod_{1\leqslant i<j\leqslant n}\sin(a_i-a_j)\sin(b_i-b_j)}{\prod_{1\leqslant i,j\leqslant n}\sin(a_i+b_j)}. \tag{B7}$$

Write out A_n explicitly as

$$A_n = \begin{vmatrix} \frac{1}{\sin(a_1+b_1)} & \frac{1}{\sin(a_1+b_2)} & \cdots & \frac{1}{\sin(a_1+b_n)} \\ \frac{1}{\sin(a_2+b_1)} & \frac{1}{\sin(a_2+b_2)} & \cdots & \frac{1}{\sin(a_2+b_n)} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{\sin(a_n+b_1)} & \frac{1}{\sin(a_n+b_2)} & \cdots & \frac{1}{\sin(a_n+b_n)} \end{vmatrix}. \tag{B8}$$

In the above determinant, multiply the last column by $\frac{-\sin b_n}{\sin b_i}$ and add to the ith column for $i = 1, \ldots, n-1$. For the element at (i, j), we have

$$\frac{1}{\sin(a_i+b_j)} + \frac{1}{\sin(a_i+b_n)}\frac{-\sin(b_n)}{\sin(b_j)} = \frac{\sin a_i \sin(b_j-b_n)}{\sin(a_i+b_j)\sin(a_i+b_n)\sin b_j}. \tag{B9}$$

Making use of this identity and extracting a common factor for each row and column, we find

$$A_n = \frac{\prod_{i=1}^{n-1}\sin(b_i-b_n)}{\prod_{j=1}^{n}\sin(a_j+b_n)} \begin{vmatrix} \frac{\sin a_1}{\sin b_1\sin(a_1+b_1)} & \frac{\sin a_1}{\sin b_2\sin(a_1+b_2)} & \cdots & 1 \\ \frac{\sin a_2}{\sin b_1\sin(a_2+b_1)} & \frac{\sin a_2}{\sin b_2\sin(a_2+b_2)} & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\sin a_n}{\sin b_1\sin(a_n+b_1)} & \frac{\sin a_n}{\sin b_2\sin(a_n+b_2)} & \cdots & 1 \end{vmatrix}. \tag{B10}$$

Subtracting the last row from all previous rows and extracting common factors, we find

$$\begin{aligned} A_n &= \frac{\prod_{i=1}^{n-1}\sin(b_i-b_n)\sin(a_i-a_n)}{\prod_{j=1}^{n}\sin(a_j+b_n)\prod_{j=1}^{n-1}\sin(a_n+b_j)} \begin{vmatrix} \frac{1}{\sin(a_1+b_1)} & \frac{1}{\sin(a_1+b_2)} & \cdots & 0 \\ \frac{1}{\sin(a_2+b_1)} & \frac{1}{\sin(a_2+b_2)} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\sin a_n}{\sin b_1\sin(a_n+b_1)} & \frac{\sin a_n}{\sin b_2\sin(a_n+b_2)} & \cdots & 1 \end{vmatrix} \\ &= \frac{\prod_{i=1}^{n-1}\sin(b_i-b_n)\sin(a_i-a_n)}{\prod_{j=1}^{n}\sin(a_j+b_n)\prod_{j=1}^{n-1}\sin(a_n+b_j)} A_{n-1}. \end{aligned} \tag{B11}$$

By mathematical recursion assumption, we have

$$A_{n-1} = \frac{\prod_{1\leqslant i<j\leqslant n-1}\sin(a_i-a_j)\sin(b_i-b_j)}{\prod_{1\leqslant i,j\leqslant n-1}\sin(a_i+b_j)}. \tag{B12}$$

Plugging Eq. (B12) into Eq. (B11), we get back Eq. (B7), which finishes the proof of Eq. (34).

APPENDIX C: ASYMPTOTIC ANALYSIS OF EQ. (44)

For $N = 2L+1$, we have an exact identity (for $N = 2L$, it is approximate),

$$\frac{1}{N\sin\theta} = \prod_{1\leqslant m\leqslant L}(\cos^2\theta - \cot^2 m\theta\, \sin^2\theta), \tag{C1}$$

so we find

$$\ln S_{r,N} = U_{r,N} + V_{r,N}, \tag{C2}$$

$$U_{r,N} = \sum_{m=1}^{r-1} m\, \ln(\cos^2\theta - \cot^2 m\theta\, \sin^2\theta), \tag{C3}$$

$$V_{r,N} = r\sum_{m=r}^{(N-1)/2} \ln(\cos^2\theta - \cot^2 m\theta\, \sin^2\theta). \tag{C4}$$

Introducing the Taylor expansion,

$$\ln(\cos^2\theta - \cot^2 m\theta\, \sin^2\theta) = \ln\left(1 - \frac{1}{4m^2}\right) - \frac{1}{3}\theta^2 - \frac{1+24m^2}{90}\theta^4 - \frac{2(1+60m^2+240m^4)}{2835}\theta^6 - \cdots, \tag{C5}$$

substituting it into Eq. (C3), and accomplishing the summation, we get

$$U_{r,N} = g_1(\alpha) + \sum_{m=1}^{r-1} m \ln\left(1 - \frac{1}{4m^2}\right) + O\left(\frac{1}{N}\right), \tag{C6}$$

where $g_1(\alpha)$ is a convergent series,

$$g_1(\alpha) = -\frac{\pi^2\alpha^2}{24} - \frac{\pi^4\alpha^4}{240} - \frac{\pi^6\alpha^6}{2268} - \frac{\pi^8\alpha^8}{21600} - \frac{\pi^{10}\alpha^{10}}{207900} - \frac{691\pi^{12}\alpha^{12}}{1393119000} - \frac{\pi^{14}\alpha^{14}}{19646550} - \frac{3617\pi^{16}\alpha^{16}}{694702008000} - \cdots. \tag{C7}$$

The second term turns out to be [29,31]

$$\sum_{m=1}^{r-1} m \ln\left(1 - \frac{1}{4m^2}\right) \approx \frac{1}{4} - \frac{1}{4}\ln r + \ln b_1, \tag{C8}$$

where $b_1 = e^{1/4}2^{1/12}A^{-3} \approx 0.645002448$; $A = 1.28242713$ is the Glaisher constant.

Likewise, by substituting Eq. (C5) into (C4) and accomplishing the summation, we get

$$V_{r,N} = g_2(\alpha) + r \sum_{m=r}^{(N-1)/2} \ln\left(1 - \frac{1}{4m^2}\right) + O\left(\frac{1}{N}\right), \tag{C9}$$

where $g_2(\alpha)$ is another convergent series,

$$g_2(\alpha) = -\frac{\pi^2}{24}\alpha(1-2\alpha) - \frac{\pi^4}{1440}\alpha[1-(2\alpha)^3] - \frac{\pi^6}{60480}\alpha[1-(2\alpha)^5] - \frac{\pi^8}{2419200}\alpha[1-(2\alpha)^7] - \frac{\pi^{10}}{95800320}\alpha[1-(2\alpha)^9]$$
$$- \frac{691\pi^{12}}{2615348736000}\alpha[1-(2\alpha)^{11}] - \frac{\pi^{14}}{149448499200}\alpha[1-(2\alpha)^{13}] - \frac{3617\pi^{16}}{21341245685760000}\alpha[1-(2\alpha)^{15}] - \cdots, \tag{C10}$$

and, as the leading order, the second term is tackled as

$$r \sum_{m=r}^{(N-1)/2} \ln\left(1 - \frac{1}{4m^2}\right) \approx -\frac{r}{4}\int_r^{(N-1)/2} \frac{1}{m^2} dm \approx -\frac{1-2\alpha}{4}. \tag{C11}$$

Compared with the traditional result, $-\frac{1}{4}$, our result shows that an extra factor $\frac{\alpha}{2}$ was dropped in the leading order in the previous works [29,31]. At last, we finish the analysis by summing up all the essential terms and writing down [just Eq. (50) in the text]

$$S(\alpha) \equiv \lim_{N\to\infty} S_{r,N} = \frac{b_1}{r^{1/4}} e^{h(\alpha)}, \tag{C12}$$

where we have defined

$$h(\alpha) = \frac{\alpha}{2} + g_1(\alpha) + g_2(\alpha). \tag{C13}$$

APPENDIX D: BETHE ANSATZ FOR HEISENBERG MODEL WITH ODD NUMBER LATTICE SITES

For completeness, in this section we briefly review the method of the Bethe ansatz. The basic idea of the Bethe ansatz is to assume that the eigenfunction can be written as a superposition of plane waves as

$$f(n_1, n_2, \ldots, n_{N_\downarrow}) = \sum_P A(P) \prod_{j=1}^{M} \left(\frac{x_{Pj}+i}{x_{Pj}-i}\right)^{n_j}. \tag{D1}$$

Here x_j for $j = 1, \ldots, N_\downarrow$ are usually called Bethe roots, which will be determined later. P denotes the permutation of Bethe roots. The requirement that $|\psi\rangle$ be an eigenstate of H^H determines the amplitude $A(P)$ in terms of Bethe roots as follows:

$$A(P) = A_0\epsilon(P)\prod_{j<l}(x_{Pj} - x_{Pl} + 2i). \tag{D2}$$

Here $\epsilon(P) = 1$ if P is an even permutation and $\epsilon(P) = -1$ if P is an odd permutation. A_0 is the overall normalization factor.

The periodic boundary condition gives rise to the following Bethe equation:

$$\left(\frac{x_j+i}{x_j-i}\right)^N = \prod_{l\neq j}\left(\frac{x_j - x_l + 2i}{x_j - x_l - 2i}\right), \tag{D3}$$

which determines the Bethe roots. To solve the above equation, it is more convenient to take the logarithm of both sides and find

$$2N \arctan x_j = 2\pi I_j + 2\sum_{l=1}^{N_\downarrow} \arctan \frac{x_j - x_l}{2}, \qquad \text{(D4)}$$

where I_j for $j = 1, \dots, N_\downarrow$ are integers if $N - N_\downarrow$ is odd and are half-odd integers if $N - N_\downarrow$ is even. All eigenfunctions of H^H can be obtained by solving Eq. (D4) with all possible choices of different sets of I_j. Substitute the solved Bethe roots into Eq. (D2) and Eq. (D1) and then the exact eigenfunction is obtained.

The ground state corresponds to the most symmetric and uniform distribution of I_j. For odd N, if $N_\downarrow = (N-1)/2$ is even, we can take the following two choices for I_j:

$$\{I_j\} = \left\{-\frac{M}{2} + 1, \dots, -1, 0, 1, \dots, \frac{M}{2}\right\},$$

$$\{I_j\} = \left\{-\frac{M}{2}, \dots, -1, 0, 1, \dots, \frac{M}{2} - 1\right\}.$$

If $N_\downarrow$ is odd, we take I_j as

$$\{I_j\} = \left\{-\frac{M}{2} + 1, \dots, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \dots, \frac{M}{2}\right\},$$

$$\{I_j\} = \left\{-\frac{M}{2}, \dots, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \dots, \frac{M}{2} - 1\right\}.$$

Note that in both cases there is a hole either located at the left end or the right end. One can verify that these two sets of I_j give the two degenerate ground states. Recall that we can flip all spins to find another two degenerate states with the same energy in the subspace with $N_\downarrow = (N+1)/2$. Therefore, the total ground state degeneracy of the antiferromagnetic Heisenberg model with odd number of sites is four, the same as the isotropic XY model. By taking one of the above sets of I_j, we numerically solve Bethe equations to obtain the Bethe roots, then plug into Eqs. (D1) and (D2) to find the ground state wave function.

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