

Multiparticle states investigation with the tensor renormalization group method

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We investigate multiparticle states of the $(1 + 1)$ d Ising Model using a spectroscopy scheme based on the transfer matrix and tensor renormalization group method. The scheme begins with computing the energy spectrum of the system from the transfer matrix estimated by the coarse-grained tensor network. The quantum number and momentum of these energy eigenstates are not *a priori* known, thus we identify them using matrix elements of an interpolating operator that is numerically computed with an impurity tensor network. Furthermore, by observing the dependence of the energy as a function of system size, we identify the number of particles of the eigenstates and obtain one-, two-, and three-particle states for a specific quantum number and momentum. From the two-particle state sector, we compute the scattering phase shift using Lüscher's formula and the wave function approach, and observe their consistency with theoretical prediction. Using the information of the two-particle scattering phase shift, we investigate the degeneracy of the two-particle states, the theoretical prediction of the three-particle finite volume energy, and also the degeneracy in the three-particle states.

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I. INTRODUCTION

The study on the multiparticle state is important for modern physics, particularly for a system that involves strong interaction such as nuclear and high energy physics. In nuclear physics, the formation of nuclei involves the two- and three-nucleon interactions. In high energy physics, multiparticle states appear during the decay processes of several hadrons such as $\rho(770)$, which mainly decays into two pions. Other examples are $\omega(782)$ and $\pi(1300)$, which mainly decay into three pions, etc. Within the framework of lattice quantum chromodynamics (LQCD), these states can be studied with non-perturbative spectroscopy calculation where the Monte Carlo algorithm is primarily applied for the computation [1–4]. Despite the success of Monte Carlo algorithms for spectroscopy calculations in LQCD, there are some difficulties that hinder the computation. A large lattice extent in the time direction is required to reduce contamination from higher eigenstates, and very high statistics are needed to suppress noise in the extraction of excited states

signals. Motivated by these issues, the tensor network has emerged as an alternative and promising method for spectroscopy calculation. The method has two approaches, i.e., the Hamiltonian approach [5–11] and the Lagrangian approach [12–44]. The spectroscopy scheme using the former approach is presented in Refs. [45–47], and the latter one is in Refs. [48,49].

In the present work, we focus on the Lagrangian approach in which the energy spectrum is extracted from the transfer matrix of the system and the estimation of this matrix is calculated using one of the tensor renormalization group algorithms [50–64], for instance, the higher order tensor renormalization group algorithm (HOTRG) [51]. The quantum number of the energy eigenstate is not *a priori* known, so we identify it with a selection rule derived from the symmetry of the system. The important quantity for the selection rule is the matrix element of an interpolating operator, which can be represented as an impurity tensor network, and then coarse grained by using HOTRG to obtain its estimate. The momentum can also be identified in a similar manner.

With this method, basically one can extract the energy spectrum of the system using only a single-time slice of the lattice, and no statistical errors are present because this method is deterministic. However, the coarse graining with HOTRG introduces systematic errors. Reference [48] showed that, for two-dimensional system, the transfer matrix estimated from a single-time slice tensor network produces eigenvalues that are closely degenerate, which

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causes large errors during the coarse-graining steps. To resolve this issue, a square tensor network is used to perform the calculation. Although this method produces reasonable results, the errors of the extracted energy spectrum increase drastically as the system size becomes larger, particularly for higher excited states. Consequently, the system sizes that we can explore are limited and the calculation is restricted to low lying-energy eigenstates.

In this paper, we introduce a new coarse-graining strategy to improve the accuracy, and reliably extract the energy of the higher excited states, which are expected to correspond to the multiparticle states. Additionally, the analysis of the dynamical properties of the two-particle state sector is also performed. We compute the phase shift of the two-particle scattering state with zero total momentum using both the finite volume energy approach based on Lüscher's formula [65–68] and the wave function approach [69–72]. We also compute the phase shift from the states with nonzero total momentum following the procedures given in Refs. [73,74], and check the consistency of the phase shift extracted from these different methods. Lastly, using the information of phase shift, we compute the two- and three-particle state dispersion relation for both zero and nonzero total momentum, and investigate the degeneracy of the energy eigenstates in these sectors.

This paper is organized as follows. The formulation of the computational scheme is given in Sec. II. At the beginning, we briefly review the transfer matrix formalism and the tensor network representation for the computation of the energy spectrum and the matrix elements for the quantum number identification in Sec. II A. After that, we explain the new strategy for the coarse graining of the tensor network in Sec. II B. We apply the scheme to (1 + 1)d Ising Model and show the numerical results in Sec. III, where the energy spectrum, quantum number, momentum, number of particles, and wave function are given in Secs. III A–III E, respectively. In Sec. III F, we present the scattering phase shift of the two-particle state sector. The phase shifts computed from the energy spectrum with Lüscher's formula in rest and moving frame are given in Sec. III F 1. Meanwhile, the phase shifts obtained from the wave function outside and inside interaction range are presented in Secs. III F 2 and III F 3, respectively. The two-particle states dispersion relation, and their degeneracy are discussed in Sec. III F 4. Moreover, the theoretical prediction of three-particle states from the dispersion relation, and discussion about their degeneracies are

presented in Secs. III G 1, and III G 2, respectively. The summary is given in the final Section. Lastly, we present the derivation of Lüscher's equation from the wave function inside the interaction range in the Appendix.

II. FORMULATION

A. Transfer matrix formulation and its tensor network representation

Let us start with a brief review of the spectroscopy scheme using transfer matrix and tensor network that we proposed in [48]. The scheme is explained in the framework of the two dimensional scalar field theory with nearest-neighbor interactions on lattice. However, its extension to higher dimensional systems is straightforward, and in principle, the scheme is also applicable to fermionic or gauge systems. The lattice action of the (1 + 1)d scalar field theory in Euclidean space time is given by

$$S[\phi] = \sum_{\mathbf{r} \in \Gamma} \left[\sum_{\mu=0}^1 \frac{1}{2} (\phi(\mathbf{r} + \hat{\mu}) - \phi(\mathbf{r}))^2 + V(\phi(\mathbf{r})) \right]. \quad (1)$$

Here, $\phi(\mathbf{r})$ is the scalar field resides on two dimensional square lattice $\mathbf{r} = (t, x) \in \Gamma$ and $\hat{\mu}$ is the unit vector for the $\mu = 0, 1$ direction, where the 0 direction (1 direction) is considered as the time (space) direction. The lattice Γ has a periodic boundary in the spatial direction, and can be defined as

$$\Gamma = \{(t, x) | t = 0, 1, 2, \dots, L_t - 1 \text{ and } x = 0, 1, 2, \dots, L_s - 1\}, \quad (2)$$

where L_t and L_s denote the lattice size in time and space direction, respectively. Note that the mass term and self-interaction term are already included in the potential $V(\phi(\mathbf{r}))$. Accordingly, the partition function of the system is given by

$$Z = \int \prod_{\mathbf{r} \in \Gamma} d\phi(\mathbf{r}) e^{-S[\phi]}. \quad (3)$$

This partition function can be reformulated in terms of the transfer matrix

$$Z = \text{Tr}[\mathcal{T}^{L_t}], \quad (4)$$

where the transfer matrix $\mathcal{T}$ [see Fig. 1(a) for the diagram] is given by [75]

$$\begin{aligned} \mathcal{T}_{\Phi\Phi} = & \left(\prod_{x=0}^{L_s-1} \exp \left[-\frac{1}{2} (\phi'_x - \phi_x)^2 - \frac{1}{4} V(\phi'_x) - \frac{1}{4} V(\phi_x) \right] \right) \left(\prod_{x=0}^{L_s-1} \exp \left[-\frac{1}{4} (\phi'_{x+1} - \phi'_x)^2 - \frac{1}{8} V(\phi'_{x+1}) - \frac{1}{8} V(\phi'_x) \right] \right) \\ & \times \left(\prod_{x=0}^{L_s-1} \exp \left[-\frac{1}{4} (\phi_{x+1} - \phi_x)^2 - \frac{1}{8} V(\phi_{x+1}) - \frac{1}{8} V(\phi_x) \right] \right), \end{aligned} \quad (5)$$

where

$$\Phi' = \{\phi'_x = \phi(t+1, x) | x = 0, 1, 2, \dots, L_s - 1\}, \quad (6)$$

$$\Phi = \{\phi_x = \phi(t, x) | x = 0, 1, 2, \dots, L_s - 1\} \quad (7)$$

are field configurations on the Euclidean time slice at $t+1$ and t . In this case, $\mathcal{T}_{\Phi'\Phi}$ is treated as a usual matrix where Φ is treated as integer-valued index for notational convenience. The diagonalization of $\mathcal{T}_{\Phi'\Phi}$ is given by

$$\mathcal{T}_{\Phi'\Phi} = \sum_{a=0}^{\infty} U_{\Phi'a} \lambda_a (U^\dagger)_{a\Phi} \iff \hat{T}|a\rangle = \lambda_a |a\rangle. \quad (8)$$

Here $U_{\Phi'a} = \langle \Phi' | a \rangle$ is the field representation of the eigenstate $|a\rangle$. The eigenvalues λ_a give us the information of the energy eigenvalues E_a of the system

$$\lambda_a = e^{-E_a} \quad \text{for } a = 0, 1, 2, 3, \dots \quad (9)$$

where $\lambda_0 \geq \lambda_1 \geq \dots$. Instead of energy E_a , the energy gaps ω_a

$$\omega_a = E_a - E_0 \quad \text{for } a = 1, 2, 3, \dots \quad (10)$$

where E_0 is the ground state energy, are more useful. Hereafter, the energy gap spectrum ω_a will be mentioned as the energy spectrum for simplicity.

The quantum number of each eigenstate $|a\rangle$ is not *a priori* known. Therefore, we identify it using matrix elements

$$\langle b | \hat{\mathcal{O}}_q | a \rangle = (U^\dagger \mathcal{O}_q U)_{ba}, \quad (11)$$

where U is the unitary matrix from Eq. (8), $\hat{\mathcal{O}}_q$ is an interpolating operator with quantum number q and $\mathcal{O}_q$ is the field representation of the interpolating operator

$$(\mathcal{O}_q)_{\Phi'\Phi} = \langle \Phi' | \hat{\mathcal{O}}_q | \Phi \rangle. \quad (12)$$

A selection rule derived from the symmetry determines the quantum number of the eigenstate $|a\rangle$. As derived in [48], the selection rule for the system with discrete symmetry is given by

$$\langle b | \hat{\mathcal{O}}_q | a \rangle \neq 0 \rightarrow q_b q q_a = 1, \quad (13)$$

where q_a, q_b are the quantum numbers for eigenstates $|a\rangle$ and $|b\rangle$, respectively. Solving Eq. (13) for known q_b and q , yields the quantum number of the state $|a\rangle$. The quantum number in systems with continuous symmetries can also be classified using a similar approach, see [48].

After presenting the formalism for computing the energy spectrum and identifying the corresponding quantum numbers, we now discuss how to compute them numerically. Because the dimensionality of transfer matrix is extremely large, we apply an approximation method to compute its eigenvalues and extract the energy spectrum, which in our case is based on tensor network techniques. To construct the tensor network representation of the transfer matrix in Eq. (5), we first decompose the transfer matrix into

$$\mathcal{T}_{\Phi'\Phi} = \sum_k Y_{\Phi'k} Y_{k\Phi}^\dagger, \quad (14)$$

where $k = \{k_x | x = 0, 1, 2, \dots, L_s - 1\}$ is a newly defined integrated index and the matrix Y is defined as

$$Y_{\Phi k} = \left(\prod_{x=0}^{L_s-1} \sum_{k_x} u_{\phi_x k_x} \sqrt{\sigma_{k_x}} \right) \left(\prod_{x=0}^{L_s-1} \exp \left[-\frac{1}{4} (\phi_{x+1} - \phi_x)^2 - \frac{1}{8} V(\phi_{x+1}) - \frac{1}{8} V(\phi_x) \right] \right). \quad (15)$$

The matrix $u_{\phi_x k_x}$ and σ_{k_x} are obtained from the eigenvalue decomposition (EVD) of the Boltzmann weight in Eq. (5) for the fields $(\phi, \phi' \in \mathbb{R})$, specifically from the temporal hopping term, namely

$$\begin{aligned} & \exp \left[-\frac{1}{2} (\phi' - \phi)^2 - \frac{1}{4} V(\phi') - \frac{1}{4} V(\phi) \right] \\ &= \sum_{k=0}^{\infty} u_{\phi'k} \sigma_k (u^\dagger)_{k\phi}. \end{aligned} \quad (16)$$

Using the matrix Y in Eq. (15), the partition function in Eq. (4) can be rewritten as

$$\begin{aligned} Z &= \text{Tr}_\Phi [\mathcal{T}^{L_t}] = \text{Tr}_\Phi [(Y Y^\dagger)^{L_t}] \\ &= \text{Tr}_k [(Y^\dagger Y)^{L_t}] = \text{Tr}_k [\mathcal{A}^{L_t}]. \end{aligned} \quad (17)$$

Here, we have defined

$$\mathcal{A} := Y^\dagger Y. \quad (18)$$

As seen in Fig. 1(b), $\mathcal{A}$ can be written as a product of rank-four tensors

$$\mathcal{A}_{kj} = \sum_{\{l\}} \prod_{x=0}^{L_s-1} A_{k_x l_x j_x l_{x-1}} \quad (19)$$

where the tensor $A_{k_x l_x j_x l_{x-1}}$ is computed by

$$A_{k_x l_x j_x l_{x-1}} := \sqrt{\sigma_{k_x} \sigma_{l_x} \sigma_{j_x} \sigma_{l_{x-1}}} \sum_{\phi_x} (u^\dagger)_{k_x \phi_x} (u^\dagger)_{l_x \phi_x} u_{\phi_x j_x} u_{\phi_x l_{x-1}}. \quad (20)$$

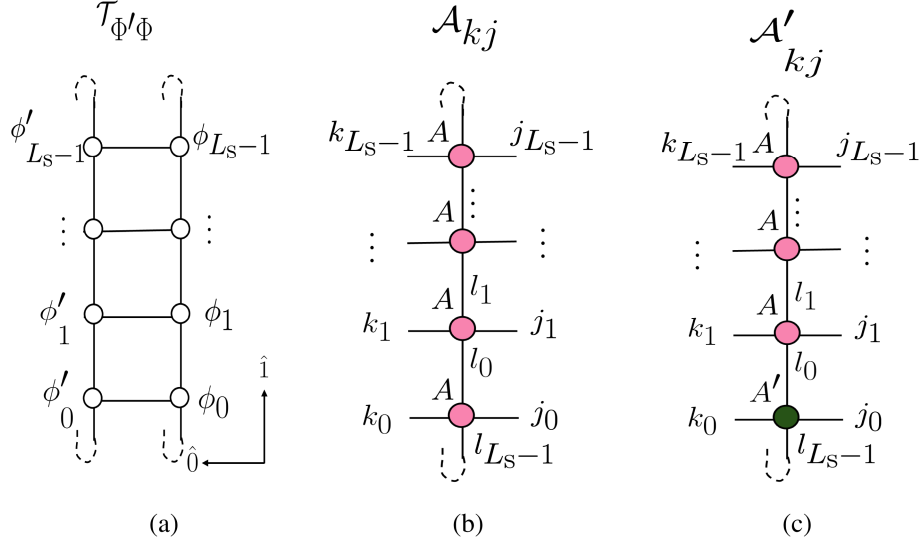


FIG. 1. Graphical image of (a) transfer matrix, (b) single-time slice tensor network, and (c) single-time slice impurity tensor network consisting of several pure tensors A and one impurity tensor A' .

The EVD of this single-time slice tensor network $\mathcal{A}_{kj}$ is given by

$$\mathcal{A}_{kj} = W_{ka} \lambda_a W_{aj}^\dagger, \quad (21)$$

where λ_a are the same eigenvalues as in Eq. (8) and W is a diagonalization matrix.

Next, we consider the matrix elements $\langle b | \hat{\mathcal{O}}_q | a \rangle$. This matrix also has very large dimensionality, so we apply the tensor network methods to approximate it as well. For this purpose, we first rewrite $\langle b | \hat{\mathcal{O}}_q | a \rangle$ in the tensor network language. The complete procedure for formulating matrix elements in terms of the tensor network is given in [48], where the final expression is given by

$$\langle b | \hat{\mathcal{O}}_q | a \rangle = (\lambda^{-m+1/2} W^\dagger \mathcal{A}^{m-1} \mathcal{A}' \mathcal{A}^m W \lambda^{-m-1/2})_{ba}. \quad (22)$$

Here, $\mathcal{A}^{m-1} \mathcal{A}' \mathcal{A}^m$ represents an impurity tensor network, and $1 \leq m \leq L_t/2$ specifies the position of $\mathcal{A}'$ within the network (see Fig. 4). In this work, we choose $m = L_t/2$. The reason for this choice is explained in Ref. [48]. Note that $\mathcal{A}'$ is the impurity version of $\mathcal{A}$, that is $\mathcal{A}' := Y^\dagger \mathcal{O}_q Y$, where Y is the matrix given in Eq. (15). For a single field $\mathcal{O}_q = \phi_x$ at lattice site x , an impurity tensor A' is defined as

$$A'_{k_x l_x j_x l_{x-1}} := \sqrt{\sigma_{k_x} \sigma_{l_x} \sigma_{j_x} \sigma_{l_{x-1}}} \sum_{\phi_x} \phi_x(u^\dagger)_{k_x \phi_x} (u^\dagger)_{l_x \phi_x} u_{\phi_x j_x} u_{\phi_x l_{x-1}}. \quad (23)$$

In Fig. 1(c) we show an image of $\mathcal{A}'$, which is composed of several pure tensors A and the single impurity tensor A' located at $x = 0$. The mathematical expression of the single-time slice impurity tensor network $\mathcal{A}'_{kj}$ shown in

terms of A and A' is given by

$$\mathcal{A}'_{kj} = \sum_{\{l\}} A'_{k_0 l_0 j_0 l_{L_S-1}} \prod_{x=1}^{L_S-1} A_{k_x l_x j_x l_{x-1}}. \quad (24)$$

B. Coarse-graining of tensor network

Here, we explain how to coarse grain the tensor network representation of transfer matrix and matrix elements derived in the previous Section using HOTRG algorithm [51]. In the following, the bond dimension of the initial tensor is denoted by χ .

It is well known that single coarse-graining iteration of HOTRG naturally reduces the tensor network size by a factor of two, thereby restricting the accessible system sizes to $L_s = 2^n$, where $n = 0, 1, 2, \dots$ is the number of coarse-graining steps. To access a wider range of spatial sizes, we prepare an initial single-time slice tensor network¹ with spatial size $L_s^{(\text{init})}$ and then embed it into the main tensor network such that the total spatial size becomes $L_s = L_s^{(\text{init})} \times 2^n$. Note that, throughout this work, we use initial tensor sizes $L_s^{(\text{init})} \in \{1, 3, 5, 7\}$.

For this purpose, we denote the tensor A in Eq. (20) as a bare tensor $A^{[0,0]}$. The size of initial tensor network is set as $L_s^{(\text{init})} = r + 1$ for $r \in \{0, 2, 4, 6\}$. As shown in Fig. 2(a), contractions are applied to the bare tensors $A^{[0,0]}$ using a HOTRG-like algorithm repeatedly until only a single tensor $A^{[r,0]}$ remains. We refer to this as the HOTRG-like algorithm because the coarse graining is applied to two different

¹The idea of constructing the initial tensor network for transfer matrix was first proposed in Ref. [76].

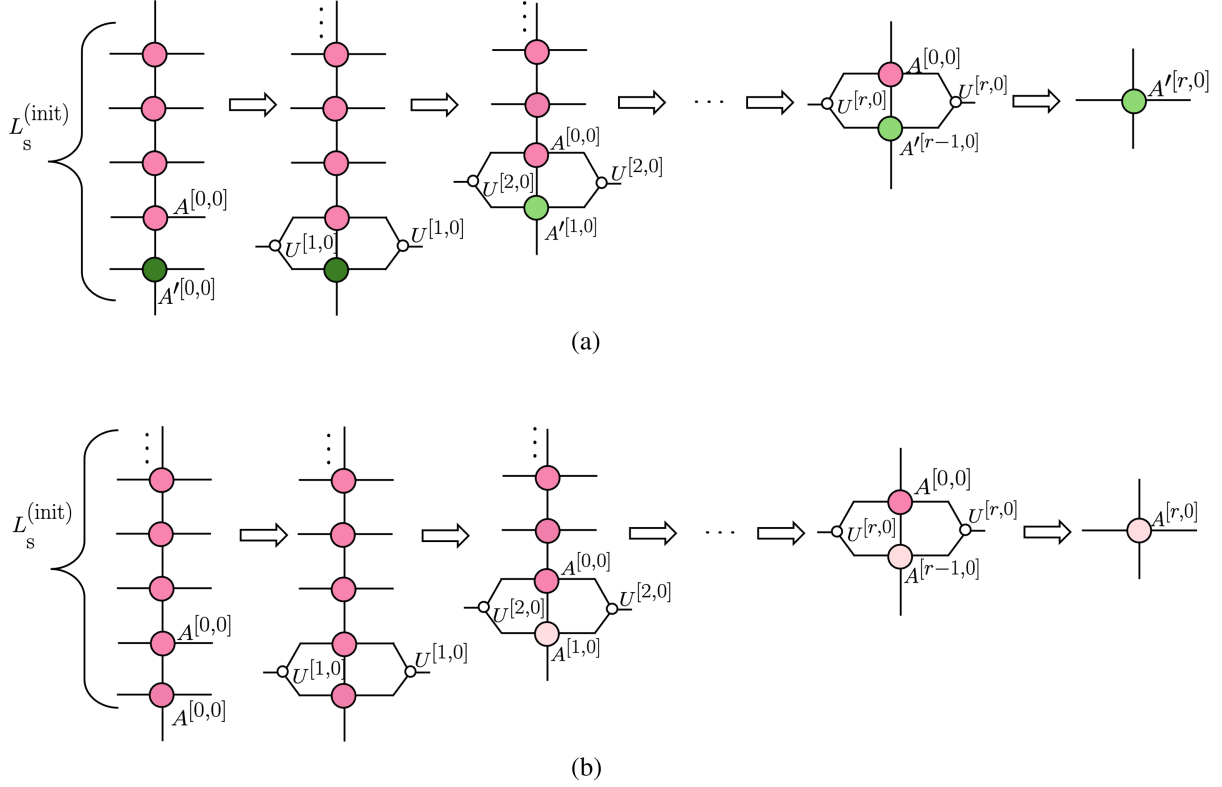


FIG. 2. (a),(b) The coarse-graining procedure for constructing the initial pure and impurity tensor networks with size $L_s^{(\text{init})} = r + 1$ for $r \in \{0, 2, 4, 6\}$. The dark pink (dark green) circle denotes the bare pure (impurity) tensor $A^{[0,0]}$ ($A'^{[0,0]}$), and the light pink (light green) circle denotes the pure (impurity) tensor network after r -th contraction, $A^{[r,0]}$ ($A'^{[r,0]}$).

tensors (see Fig. 2), although the procedure is essentially the same as in the standard HOTRG algorithm. To be concrete, a single coarse-graining step that produces the new tensor $A^{[s,0]}$ from the previously coarse-grained tensor $A^{[s-1,0]}$ is given by

$$A_{c_0 a_1 b_0 a_0}^{[s,0]} = c_0 \text{---} U^{[s,0]} \text{---} A^{[0,0]} \text{---} b_0 \text{---} A^{[s-1,0]} \text{---} a_0 \quad (s = 1, 2, \dots, r). \quad (25)$$

For $s = 1$, $A^{[s-1,0]}$ corresponds to the bare tensor. The tensor $U^{[s,0]}$ in Eq. (25) is an isometry that is computed from the EVD of the following self-adjoint matrix

$$M_{(k_0 k_1, k'_0 k'_1)}^{[s,0]} = \begin{array}{c} \text{Diagram showing the contraction of } A^{[0,0]} \text{ and } A^{[s-1,0]} \text{ tensors with indices } k_1, k'_1, k_0, k'_0. \end{array} \quad (26)$$

Applying EVD and truncating the eigenvalues of $M_{(k_0 k_1, k'_0 k'_1)}^{[s,0]}$ yields

$$M_{(k_0 k_1, k'_0 k'_1)}^{[s,0]} \approx \sum_{c_0=0}^{\chi} U^{[s,0]}_{k_0} \sigma_{c_0} U^{[s,0]}_{k'_0} \quad (27)$$

where $U^{[s,0]}$ is the isometry and σ_{c_0} are the eigenvalues of M that are truncated up to the cutoff bond dimension χ . See [51] for a complete description of the isometry.

After completing the coarse-graining of the initial tensor network with size $L_s^{(\text{init})}$, we obtain the tensor $A^{[r,0]}$. As mentioned earlier, we embed this tensor into the main tensor network, which then consists of $2^p \times 2^n$ tensors $A^{[r,0]}$, as illustrated in Fig. 3. Accordingly, the total size of the main tensor network is $L_t \times L_s = 2^p \times (L_s^{(\text{init})} \times 2^n)$. The coarse graining of this network is performed using the standard HOTRG algorithm [51], where the new tensor $A^{[r,i]}$ for $i = 1, 2, \dots, n$ is obtained from previously coarse-grained tensors $A^{[r,i-1]}$ by coarse graining for the time and spaces direction.

An important point to note is that, p and n do not only determine the size of tensor network, but also represent the

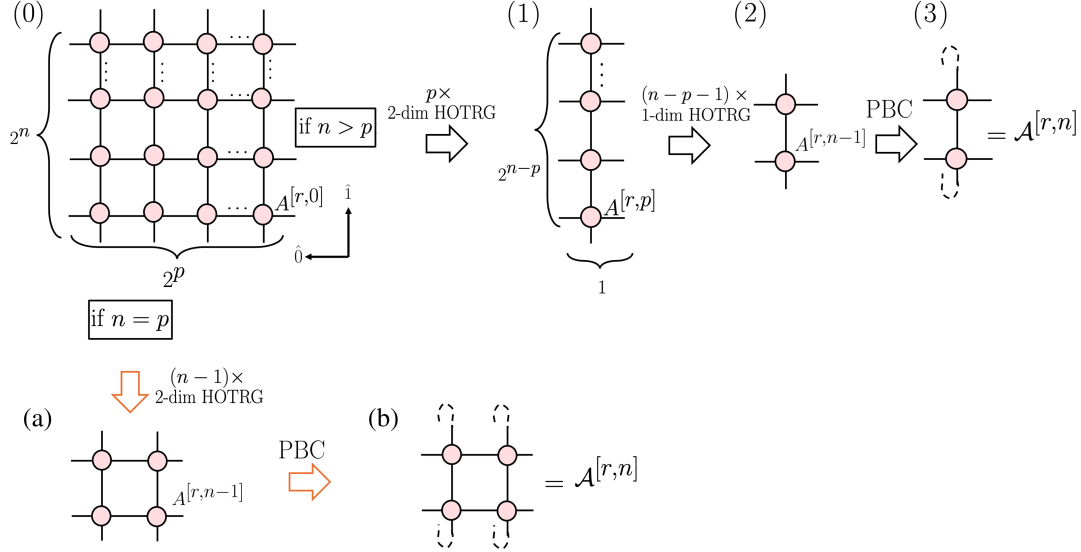


FIG. 3. Coarse-graining procedure of the main tensor network using HOTRG. The procedures (0)–(3) corresponds to the case $n > p$, while the procedures (0)–(b) apply to the case $n = p$. See the main text for detail descriptions.

number of coarse graining steps in the time and spatial directions, respectively. These values are chosen such that

$$n \geq p. \quad (28)$$

As illustrated in Fig. 3, when $n > p$, the coarse graining procedure is as follows: (1) Apply p coarse-graining iterations in both directions using two-dimensional HOTRG. (2) Continue with $(n - p - 1)$ coarse-graining iterations in the spatial direction using the one-dimensional HOTRG. (3) Perform an exact contraction to the last two remained tensors $A^{[r,n-1]}$ with the periodic boundary condition (PBC), obtaining

$$(\mathcal{A}^{L_t})_{kj} \approx \sum_{l_0, l_1} A_{k_0 l_0 j_0 l_1}^{[r,n-1]} A_{k_1 l_1 j_1 l_0}^{[r,n-1]} =: \mathcal{A}_{k_0 k_1, j_0 j_1}^{[r,n]}. \quad (29)$$

Meanwhile, the coarse graining procedure when $n = p$ is as follows: (a) Apply $(n - 1)$ coarse graining iterations in both directions using the two-dimensional HOTRG. (b) Perform an exact contraction to the last four remained tensors with PBC, resulting in

$$\begin{aligned} (\mathcal{A}^{L_t})_{kj} &\approx \sum_{l_0, l_1, m_0, m_1, n_0, n_1} A_{k_0 l_0 n_0 l_1}^{[r,n-1]} A_{k_1 l_1 n_1 l_0}^{[r,n-1]} A_{n_0 m_0 j_0 m_1}^{[r,n-1]} A_{n_1 m_1 j_1 m_0}^{[r,n-1]} \\ &=: \mathcal{A}_{k_0 k_1, j_0 j_1}^{[r,n]}. \end{aligned} \quad (30)$$

Subsequently, we apply the EVD to $\mathcal{A}^{[r,n]}$ as

$$\mathcal{A}^{[r,n]} = W^{[r,n]} \lambda^{[r,n]} W^{[r,n]\dagger}, \quad (31)$$

where $W^{[r,n]}$ is a unitary matrix that approximates W in Eq. (21) and $\lambda^{[r,n]}$ denotes the numerical eigenvalues. These

are related to the eigenvalues of $\mathcal{A}$ in Eq. (21) by

$$\lambda_a \approx (\lambda_a^{[r,n]})^{1/L_t}. \quad (32)$$

Finally, the estimated energy spectrum is given by

$$\omega_a \approx \frac{1}{L_t} \log \left(\frac{\lambda_0^{[r,n]}}{\lambda_a^{[r,n]}} \right) =: \omega_a^{[\text{hotrg}]} \quad \text{for } a = 1, 2, 3, \dots \quad (33)$$

Next, we explain the coarse graining procedure for the impurity tensor network $\mathcal{A}^{m-1} \mathcal{A}' \mathcal{A}^m$ in Eq. (22). Similar to the pure tensor case, we begin by preparing the initial impurity tensor network. The bare impurity tensor is denoted by $A'^{[0,0]} = A'$. To obtain the s -th coarse-grained impurity tensor $A'^{[s,0]}$, we perform

$$A'^{[s,0]}_{c_0 a_1 b_0 a_0} = c_0 \text{---} U^{[s,0]} \text{---} a_1 \text{---} A'^{[0,0]} \text{---} b_0 \text{---} A'^{[s-1,0]} \text{---} a_0, \quad (s = 1, 2, \dots, r) \quad (34)$$

where $A'^{[s-1,0]}$ is the previously coarse grained impurity tensor, and $U^{[s,0]}$ is the same isometry with the pure tensor case obtained from Eqs. (26) and (27). After r coarse-graining iterations, we obtain $A'^{[r,0]}$, which is then inserted to the main impurity tensor network, as shown in Fig. 4. The new tensor $A'^{[r,i]}$ in this main impurity tensor network is obtained from the previous tensors $A'^{[r,i-1]}$ and $A^{[r,i-1]}$. As in the pure tensor case, when $n > p$, the coarse

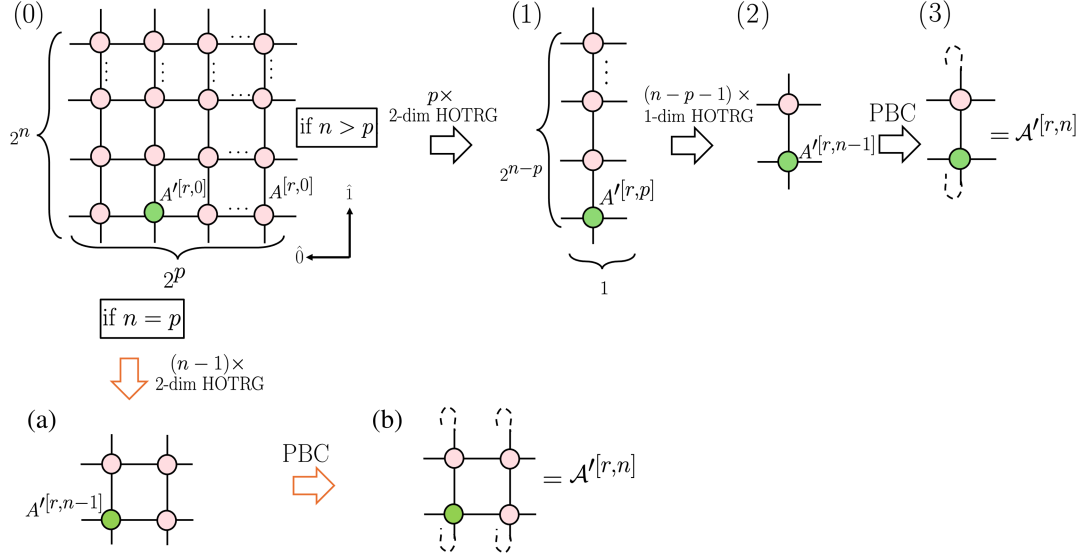


FIG. 4. Coarse-graining procedure for the impurity tensor network $\mathcal{A}^{m-1}\mathcal{A}'\mathcal{A}^m$ with $m = 2^{p-1}$. Procedure (0)–(3) is for $n > p$ while procedure (0)–(b) is for $n = p$.

graining of the impurity tensor network is carried out according to the procedure (0)–(3) shown in Fig. 4. In the last step, we perform an exact contraction for the remaining one pure tensor and one impurity tensor along with PBC, and obtain the estimate of $\mathcal{A}^{m-1}\mathcal{A}'\mathcal{A}^m$, that is

$$(\mathcal{A}^{m-1}\mathcal{A}'\mathcal{A}^m)_{kj} \approx \sum_{l_0, l_1} A'_{k_0 l_0 j_0 l_1} A_{k_1 l_1 j_1 l_0}^{[r, n-1]} =: \mathcal{A}'_{k_0 k_1, j_0 j_1}^{[r, n]}. \quad (35)$$

On the other hand, when $n = p$, we follow the procedure (0)–(b). In the final step, an exact contraction of one impurity tensor and three pure tensors is performed to obtain

$$\begin{aligned} (\mathcal{A}^{m-1}\mathcal{A}'\mathcal{A}^m)_{kj} &\approx \sum_{l_0, l_1, m_0, m_1, n_0, n_1} A_{k_0 l_0 n_0 l_1}^{[r, n-1]} A_{k_1 l_1 n_1 l_0}^{[r, n-1]} A_{n_0 m_0 j_0 m_1}^{[r, n-1]} A_{n_1 m_1 j_1 m_0}^{[r, n-1]} \\ &=: \mathcal{A}'_{k_0 k_1, j_0 j_1}^{[r, n]}. \end{aligned} \quad (36)$$

After the building blocks of matrix elements have been estimated, we compute the approximate matrix elements given in Eq. (22), using the following expression

$$\begin{aligned} \langle b | \hat{\mathcal{O}}_q | a \rangle &\approx ((\lambda^{[r, n]})^{-(m-1/2)/L_t} W^{[r, n] \dagger} \mathcal{A}'^{[r, n]} W^{[r, n]} (\lambda^{[r, n]})^{-(m+1/2)/L_t})_{ba} \\ &=: \langle b | \hat{\mathcal{O}}_q | a \rangle^{\text{[hotrg]}}. \end{aligned} \quad (37)$$

III. NUMERICAL RESULTS

In this Section, we demonstrate the spectroscopy technique to investigate the multiparticle states of the (1 + 1)d Ising model under PBC with no external magnetic field.

The partition function of the model is given by

$$Z = \sum_{\{s\}} e^{-\frac{1}{T}H} \quad (38)$$

where T is the temperature, H is the Hamiltonian of the system that is given by

$$H[s] = -J \sum_{\mathbf{r} \in \Gamma} \sum_{\mu=0}^1 s(\mathbf{r} + \hat{\mu}) s(\mathbf{r}), \quad (39)$$

where $s = \pm 1$ and J is set to be unity. The initial bare tensor $A^{[0,0]}$ of this model can be written as [77]

$$A_{abcd}^{[0,0]} = \sqrt{\sigma_a \sigma_b \sigma_c \sigma_d} \sum_{s=\pm 1} (u^\dagger)_{as} (u^\dagger)_{bs} u_{sc} u_{sd} \quad (40)$$

where u and σ are obtained from the SVD of the Boltzmann factor in the partition function, that is

$$e^{\frac{1}{T}s's} = \sum_{k=1}^2 u_{s'k} \sigma_k (u^\dagger)_{ks}. \quad (41)$$

The details can be found in Ref. [48]. In this work, the temperature of the system is fixed at $T = 2.44$, which lies in the symmetric phase.

A. Energy spectrum

In [48], a square tensor network was employed for all calculations. Using this setup, we were able to investigate the spectrum up to system size $L_s = 64$, where the highest excited state for which the quantum numbers are correctly identified corresponds to eigenstate number $a = 20$,

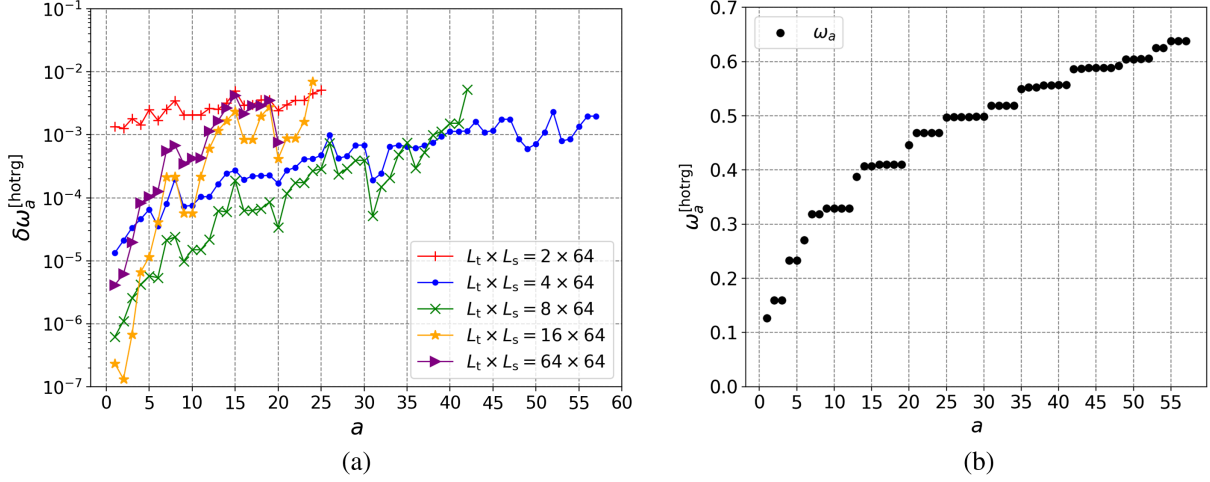


FIG. 5. (a) Relative error of the energy spectrum $\omega_a^{[\text{hotrg}]}$ for system size $L_s = 64$ computed with $\chi = 80$ and $L_t = 2, 4, 8, 16, 64$. (b) The energy spectrum $\omega_a^{[\text{hotrg}]}$ for system size $L_s = 64$, computed using HOTRG with $\chi = 80$ and $L_t = 4$.

and the error in the energy spectrum is of order $O(10^{-3})$. In the present work, we slightly modify the coarse-graining strategy to improve the accuracy of the calculations, thereby enabling access to higher eigenstates and larger system sizes. Specifically, we compute the spectrum at fixed L_s while varying system size in time direction $L_t = 2, 4, \dots, L_s$, where $L_t = L_s$ correspond to a square tensor network. The case $L_t = 1$ is excluded, as it was demonstrated in Ref. [48] that this choice leads to large numerical error.

We compute $\omega_a^{[\text{hotrg}]}$ using Eq. (33) for $L_s = 64$ and $L_t = 2, 4, 8, 16, 64$, following the procedure introduced in Sec. II B. As shown in Fig. 5(a), the tensor network with $L_t = 4, 8$ yields smaller relative error, $\delta\omega_a = \left| \frac{\omega_a^{[\text{hotrg}]} - \omega_a^{[\text{exact}]}}{\omega_a^{[\text{exact}]}} \right|$, compared to other choices $L_t = 2, 16, 64$. Here, the exact spectrum $\omega_a^{[\text{exact}]}$ is computed using Kaufman's formula [78], see the Appendix of Ref. [48] for the concise summary. There are two main reasons why $L_t = 4, 8$ produce relatively smaller errors compared to the other choices $L_t = 2, 16, 64$. First, the number of the coarse-graining steps required for $L_t = 4, 8$ is smaller than for $L_t = 16, 64$ resulting in a smaller accumulated coarse-graining error. Second, the eigenvalues of the transfer matrix tend to be more degenerate for smaller L_t , particularly when L_s is large, which leads to large errors after each coarse-graining step. This explains why $L_t = 4, 8$ yield smaller errors compared to $L_t = 2$. Furthermore, when comparing the results for $L_t = 4$ and $L_t = 8$, we observe that the low-lying eigenstates are determined more accurately for $L_t = 8$, whereas the higher eigenstates exhibit smaller error for $L_t = 4$. Since each choice, $L_t = 4, 8$ has its own advantages and disadvantages, we employ both in the computations presented in this paper. In Fig. 5(b), we present the energy spectrum $\omega_a^{[\text{hotrg}]}$ of the system for $L_s = 64$ computed using $\chi = 80$ and $L_t = 4$. In principle, our scheme allows the extraction of $\omega_a^{[\text{hotrg}]}$ up to $a = \chi^2$. However, we only

present the result for which the numerical errors are in order $O(10^{-3})$. For the case $L_s = 64$, $L_t = 4$ and $\chi = 80$, these correspond to the eigenstates $a = 0-57$.

Next, we examine how the relative error of the energy spectrum changes over different cutoff bond dimension. We compute the energy spectrum for $L_s = 64$ and $L_t = 4, 8$, using $\chi = 70, 80, 90$, and present the results in Fig. 6. From the figure, we clearly observe that the relative error decreases as χ increases for both $L_t = 4, 8$, as expected. Furthermore, the figure also indicates that, for $L_s = 64$, as the cutoff bond dimension is increased, the crossover between errors for $L_t = 4$ and $L_t = 8$ moves toward larger values of a . This trend can be understood by noting that the eigenvalues of transfer matrix computed with $L_t = 4$ are more dense than those computed with $L_t = 8$. Usually in tensor network calculation, such closely degenerate structure causes large truncation error. Therefore, as the cutoff bond dimension increases, the reduction in the relative error is smaller for $L_t = 4$ than for $L_t = 8$. Consequently,

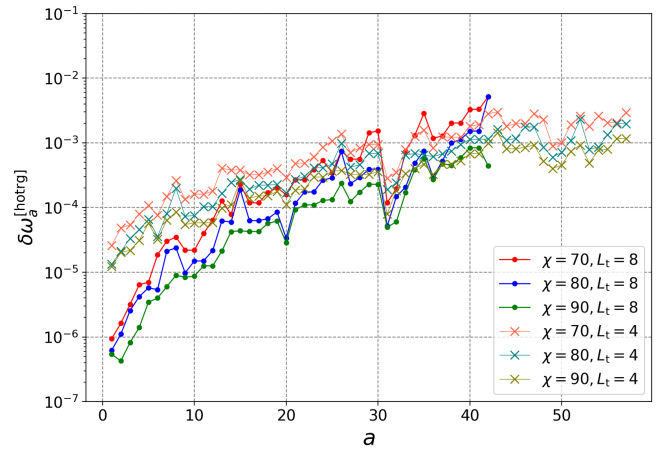


FIG. 6. Relative errors of energy spectrum for $L_s = 64$, computed with $\chi = 70, 80, 90$ and $L_t = 4, 8$.

the intersection of the errors for $L_t = 4$ and $L_t = 8$ tend to shift toward larger values of a as the bond dimension is increased.

B. Quantum number

One of the quantum numbers for $(1+1)$ d Ising model is $q = \{+1, -1\}$ which arises from the internal $\mathbb{Z}_2$ symmetry of the spin field. To classify the eigenstates according to this quantum number, we compute matrix elements of a spin field operator $\hat{s}_x$ (we use $\hat{s}_0$ at $x = 0$ in practice), namely $\langle \Omega | \hat{s}_x | a \rangle$ where $\langle \Omega |$ is the ground state whose quantum number is $q_\Omega = +1$. From the selection rule of the discrete symmetry given in Eq. (13), if $\langle \Omega | \hat{s}_0 | a \rangle \neq 0$, then the eigenstate $|a\rangle$ has a quantum number $q_a = -1$. To estimate the matrix elements, we coarse grain the corresponding impurity tensor network for $L_s = 64$ and $L_t = 4, 8$ (with the impurity placed at $m = 2, 4$, respectively), using $\chi = 80$, and substitute the result into Eq. (37). We present the energy spectrum $\omega_a^{[\text{hotrg}]}$ previously shown in Fig. 5(b) with the additional corresponding quantum number in the upper panel of Fig. 7. The quantum number classification is based on $|\langle \Omega | \hat{s}_0 | a \rangle^{[\text{hotrg}]}|$ shown in the middle panel. Meanwhile, the bottom panel displays the exact quantum number for comparison, computed following Ref. [78]. From the figures, using the matrix elements obtained with $L_t = 4$, we can correctly identify the quantum number for $L_s = 64$

up to $a = 57$, whereas those obtained with $L_t = 8$ are accurate only up to $a = 42$. In general, these results indicate that, by using tensor network with $L_t = 4, 8$, we are able to identify more higher-energy eigenstates correctly compared to the previous results reported in Refs. [48,49] using square lattice.

C. Momentum

The momentum of the eigenstate $|a\rangle$ in $q = -1$ sector can be identified by computing the matrix elements of an operator with momentum P

$$\langle \Omega | \hat{O}_1(P) | a \rangle, \quad (42)$$

where

$$\hat{O}_1(P) = \frac{1}{L_s} \sum_{x=0}^{L_s-1} \hat{s}_x e^{-iPx} \quad (43)$$

and $P = 2\pi n/L_s$ is the discrete momentum with $n = 0, 1, 2, \dots, L_s - 1$. The selection rule for momentum states that for a fixed P , if the following condition

$$\langle \Omega | \hat{O}_1(P) | a \rangle \approx \langle \Omega | \hat{O}_1(P) | a \rangle^{[\text{hotrg}]} \neq 0 \quad (44)$$

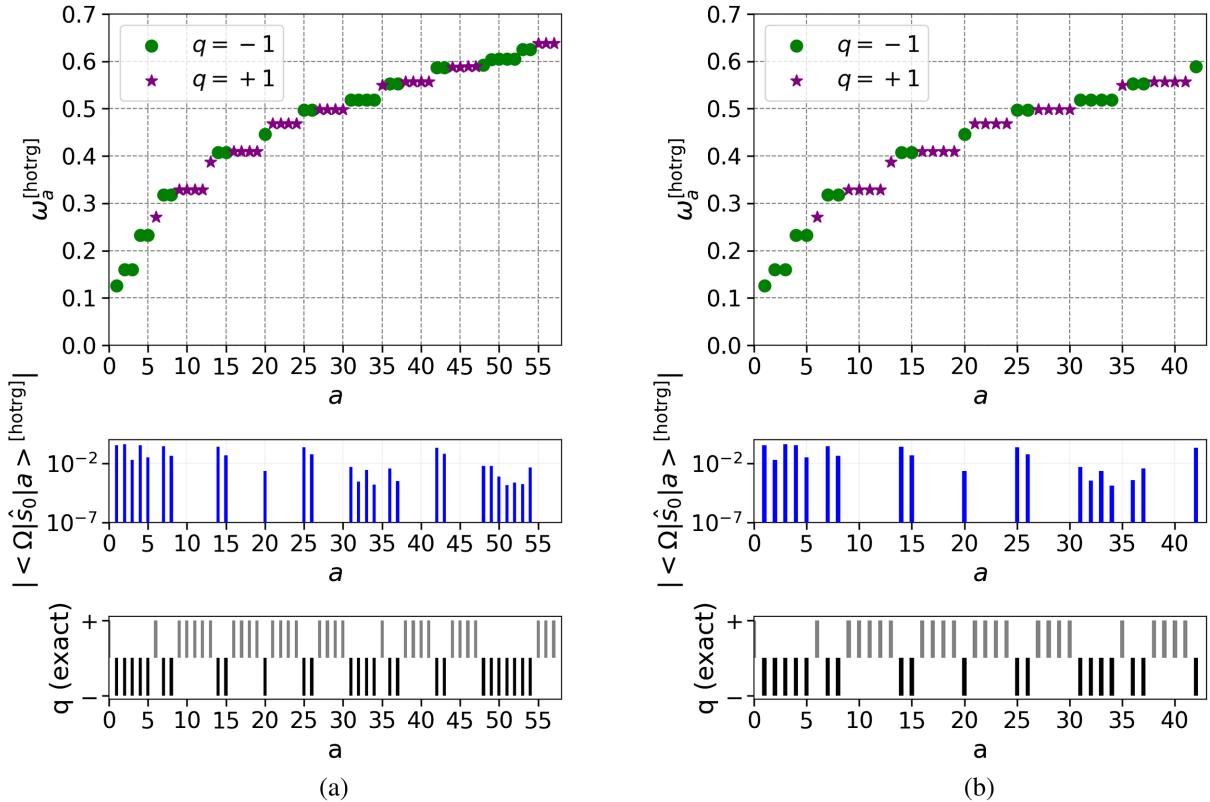


FIG. 7. Energy spectrum $\omega_a^{[\text{hotrg}]}$ and absolute value of matrix elements $|\langle \Omega | \hat{s}_0 | a \rangle^{[\text{hotrg}]}|$ for quantum number classification, together with the exact quantum number as comparison for $L_s = 64$ computed with $\chi = 80$ and using (a) $L_t = 4$ and (b) $L_t = 8$.

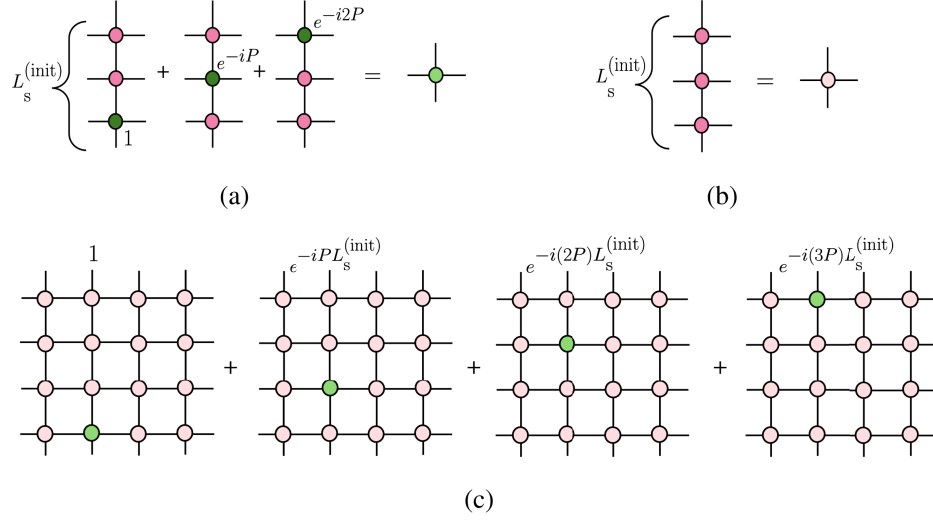


FIG. 8. (a) Initial tensor network representation with size $L_s^{(\text{init})} = 3$ for $\hat{O}_1(P)$ denoted by $A'^{[2,0]}$ (light green circle), which is constructed from one bare impurity tensor $A'^{[0,0]}$ (dark green circle) with a proper momentum factor, and two bare pure tensors (dark pink circle). (b) Initial pure tensor network (light pink circle) constructed from three bare pure tensors. (c) The main impurity tensor network with total size $L_s = L_s^{(\text{init})} \times 4$ for computing $\langle \Omega | \hat{O}_1(P) | a \rangle$.

is satisfied, then the eigenstate $|a\rangle$ carries the momentum P . In Fig. 8, we show the impurity tensor network diagram corresponding to the operator $\hat{O}_1(P)$. These networks are then coarse grained to obtain $\langle \Omega | \hat{O}_1(P) | a \rangle^{\text{[hotrg]}}$.

Table I lists the absolute values of the matrix elements $|\langle \Omega | \hat{O}_1(P) | a \rangle^{\text{[hotrg]}}|$ for the system size $L_s = 64$ computed with $L_t = 4$ and $\chi = 80$, which are used to identify momentum in $q = -1$ sector together with the selection rule in Eq. (44). For this identification, we treat $|\langle \Omega | \hat{O}_1(P) | a \rangle^{\text{[hotrg]}}| < 10^{-6}$ as zero. However, some matrix elements take values of order $O(10^{-6})$ and $O(10^{-5})$. To clarify the behavior of these values, we compute the matrix elements using a larger bond dimension, $\chi = 120$, and observe that these values decrease, indicating that they are not signals but instead arise from coarse-graining errors.

On the other hand, when the matrix elements are of order $O(10^{-4})$, we regard them as a signal if they remain consistent or increase for the larger bond dimension $\chi = 120$, and we regard them as an error if their values decrease. As one example, eigenstates $a = 31\text{--}34$ have nonzero values of order $O(10^{-4})$ at three different absolute value total momenta, $|P| = 2\pi/L_s$, $6\pi/L_s$, and $10\pi/L_s$. In this case, we conclude that the nonzero values appearing at $|P| = 10\pi/L_s$ are fake signals, because the values decrease when $\chi = 120$. With this selection rule, we can clearly classify the momentum $|P| = 0\text{--}12\pi/L_s$ of the energy eigenstates when the states are nondegenerate and twofold degenerate. For fourfold degenerate energy, for instance, the corresponding eigenstates $a = 31\text{--}34$ are associated with two different absolute total momenta, $|P| = 2\pi/L_s$ and $6\pi/L_s$. In this case, the eigenstates may be described by linear combination of these corresponding momenta.

Accordingly, the operator associated with each momentum can have non-zero overlap with the four states, leading to nonzero matrix elements at both absolute momenta $|P| = 2\pi/L_s, 6\pi/L_s$.

Next, we examine the relation between the numerical energy and momentum and compare it with both continuum dispersion relation of the one-particle state

$$\omega_1^{\text{cont}} = \sqrt{m^2 + P^2} \quad (45)$$

and the lattice dispersion relation

$$\omega_1^{\text{lat}} = \cosh^{-1}(1 - \cos P + \cosh m). \quad (46)$$

Here, m denotes the exact rest mass at $T = 2.44$ in the large volume limit,

$$m = 0.12621870. \quad (47)$$

The number of particles of the eigenstates in $q = -1$ sector will be investigated in Sec. III D. But here, by comparing with tensor network results and the one-particle dispersion relation, we roughly try to identify the one-particle state. From such identification, among all eigenstates listed in Table I for $L_s = 64$, state numbers $a = 1, 2, 3, 4, 5, 7, 8, 14, 15, 25, 26, 42, 43$ are categorized as the one-particle state (see Fig. 9). On the other hand, it can be checked that the remaining states do not fit the one-particle dispersion relation (see Fig. 9); in fact, they follow the three-particle state dispersion relation, as will be explained in Sec. III G.

In addition, we perform the same calculation of energy spectrum and the momentum identification for other system

TABLE I. Absolute value of matrix elements $|\langle \Omega | \hat{\mathcal{O}}_1(P) | a \rangle^{\text{[hotrg]}}|$ with $|P| = 0 - 12\pi/L_s$ and $L_s = 64$ computed using $\chi = 80$ and $L_t = 4$ for eigenstate $|a\rangle$ in $q = -1$ sector.

	a								
P	0	$2\pi/L_s$	$4\pi/L_s$	$6\pi/L_s$	$8\pi/L_s$	$10\pi/L_s$	$12\pi/L_s$	$ P $	$\omega_a^{\text{[hotrg]}}$
1	0.316100	$<10^{-6}$	0.000001	$<10^{-6}$	$<10^{-6}$	$<10^{-6}$	0.000001	0	0.126232
2	$<10^{-6}$	0.198509	$<10^{-6}$	0.000001	$<10^{-6}$	$<10^{-6}$	$<10^{-6}$	$2\pi/L_s$	0.159791
3	$<10^{-6}$	0.198503	$<10^{-6}$	0.000009	$<10^{-6}$	0.000009	$<10^{-6}$	$2\pi/L_s$	0.159793
4	0.000006	$<10^{-6}$	0.164112	$<10^{-6}$	0.000002	$<10^{-6}$	0.000004	$4\pi/L_s$	0.232696
5	$<10^{-6}$	$<10^{-6}$	0.164106	$<10^{-6}$	0.000015	$<10^{-6}$	0.000012	$4\pi/L_s$	0.2327
7	$<10^{-6}$	0.000006	$<10^{-6}$	0.139802	$<10^{-6}$	0.000011	$<10^{-6}$	$6\pi/L_s$	0.31818
8	$<10^{-6}$	0.000010	$<10^{-6}$	0.139800	$<10^{-6}$	0.000056	$<10^{-6}$	$6\pi/L_s$	0.318218
14	0.000002	$<10^{-6}$	0.000009	$<10^{-6}$	0.122905	$<10^{-6}$	0.000023	$8\pi/L_s$	0.407404
15	$<10^{-6}$	$<10^{-6}$	0.000017	$<10^{-6}$	0.122902	$<10^{-6}$	0.000067	$8\pi/L_s$	0.407415
20	0.002199	$<10^{-6}$	0.000005	$<10^{-6}$	0.000019	$<10^{-6}$	0.000008	0	0.445858
25	$<10^{-6}$	0.000003	$<10^{-6}$	0.000017	$<10^{-6}$	0.110530	$<10^{-6}$	$10\pi/L_s$	0.497221
26	$<10^{-6}$	0.000002	$<10^{-6}$	0.000068	$<10^{-6}$	0.110537	$<10^{-6}$	$10\pi/L_s$	0.497475
31	$<10^{-6}$	0.001747	$<10^{-6}$	0.000590	$<10^{-6}$	0.000003	$<10^{-6}$	$2\pi/L_s, 6\pi/L_s$	0.51878
32	$<10^{-6}$	0.000840	$<10^{-6}$	0.000777	$<10^{-6}$	0.000059	$<10^{-6}$	$2\pi/L_s, 6\pi/L_s$	0.518806
33	$<10^{-6}$	0.001749	$<10^{-6}$	0.000576	$<10^{-6}$	0.000194	$<10^{-6}$	$2\pi/L_s, 6\pi/L_s$	0.519017
34	$<10^{-6}$	0.002347	$<10^{-6}$	0.000303	$<10^{-6}$	0.000002	$<10^{-6}$	$2\pi/L_s, 6\pi/L_s$	0.519035
36	0.000015	$<10^{-6}$	0.001822	$<10^{-6}$	0.000002	$<10^{-6}$	0.000006	$4\pi/L_s$	0.552576
37	$<10^{-6}$	$<10^{-6}$	0.001776	$<10^{-6}$	0.000001	$<10^{-6}$	0.000090	$4\pi/L_s$	0.552611
42	0.000018	$<10^{-6}$	0.000016	$<10^{-6}$	0.000017	$<10^{-6}$	0.101022	$12\pi/L_s$	0.586424
43	$<10^{-6}$	$<10^{-6}$	0.000004	$<10^{-6}$	0.000083	$<10^{-6}$	0.101045	$12\pi/L_s$	0.586699
48	0.005158	$<10^{-6}$	0.000009	$<10^{-6}$	0.000055	$<10^{-6}$	0.000240	0	0.592084
49	0.000065	$<10^{-6}$	0.002497	$<10^{-6}$	0.000585	$<10^{-6}$	0.000219	$4\pi/L_s, 8\pi/L_s$	0.604513
50	$<10^{-6}$	$<10^{-6}$	0.001916	$<10^{-6}$	0.000979	$<10^{-6}$	0.000018	$4\pi/L_s, 8\pi/L_s$	0.604581
51	0.000014	$<10^{-6}$	0.001231	$<10^{-6}$	0.001279	$<10^{-6}$	0.000082	$4\pi/L_s, 8\pi/L_s$	0.604808
52	$<10^{-6}$	$<10^{-6}$	0.001949	$<10^{-6}$	0.000984	$<10^{-6}$	0.000440	$4\pi/L_s, 8\pi/L_s$	0.605546
53	$<10^{-6}$	0.002032	$<10^{-6}$	0.000050	$<10^{-6}$	0.000014	$<10^{-6}$	$2\pi/L_s$	0.625633
54	$<10^{-6}$	0.002014	$<10^{-6}$	0.000051	$<10^{-6}$	0.000014	$<10^{-6}$	$2\pi/L_s$	0.625672

sizes $L_s = 8-112$, and present only data that follow the one-particle dispersion relation in Fig. 10. Note that, the one-particle energy eigenstates with nonzero momentum are twofold degenerate, sharing the same absolute momentum. For example, the eigenstate numbers $a = 2, 3$ of $L_s = 64$ both have $|P| = 2\pi/L_s$; see Fig. 7 and Table I. However, this degeneracy is slightly broken because of the truncation effect, which can be reduced by increasing the cutoff bond dimension. We take the average of the corresponding energy ω and plot these average values in Fig. 10. From the figure, we observe that the one-particle state data agree well with both dispersion relations at low-momentum region, while at higher momentum, the data are well described by the lattice dispersion relation as expected.

Next, we move to the identification of the momentum for the $q = +1$ sector. In this case, we compute matrix elements

$$\langle \Omega | \hat{\mathcal{O}}_2(P, p) | a \rangle \quad (48)$$

where

$$\hat{\mathcal{O}}_2(P, p) = \frac{1}{L_s^2} \sum_{x_1, x_2} \hat{s}_{x_1} \hat{s}_{x_2} e^{-ip_1 x_1} e^{-ip_2 x_2} \quad (49)$$

and p_j ($j = 1, 2$) are the discrete momentum $p_j = \frac{2\pi n_j}{L_s}$ with $n_j = 0, 1, 2, \dots, L_s - 1$. The total momentum is given by $P = p_1 + p_2$, whose values are discrete

$$P = \frac{2\pi d}{L_s} \quad (50)$$

with $d = 0, 1, 2, \dots, L_s - 1$, and

$$p = (p_1 - p_2)/2 \quad (51)$$

is the relative momentum.² For a fixed total momentum P , if the matrix element is nonzero

$$\langle \Omega | \hat{\mathcal{O}}_2(P, p) | a \rangle \neq 0 \quad (52)$$

²In our calculation, we use the relative momentum $p = P/2$.

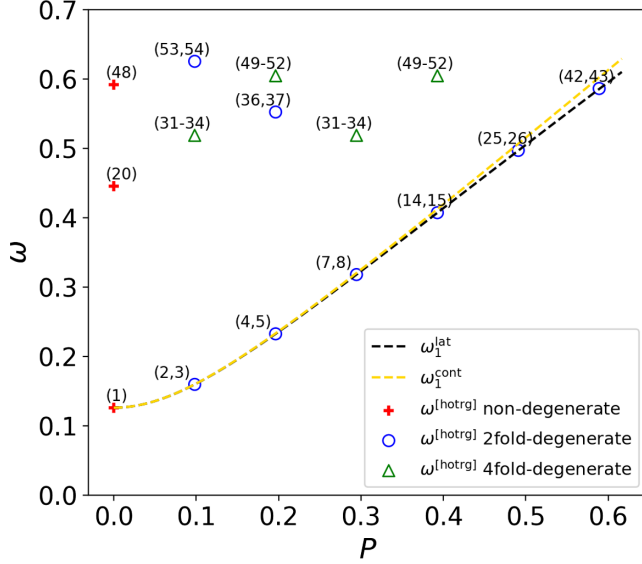


FIG. 9. Energy spectrum ω for $q = -1$ sector as a function of P for $L_s = 64$ computed with $L_t = 4$ and $\chi = 80$. The numbers in parentheses are the energy-level ordering, while the dashed lines are one-particle dispersion relation in Eqs. (45) and (46).

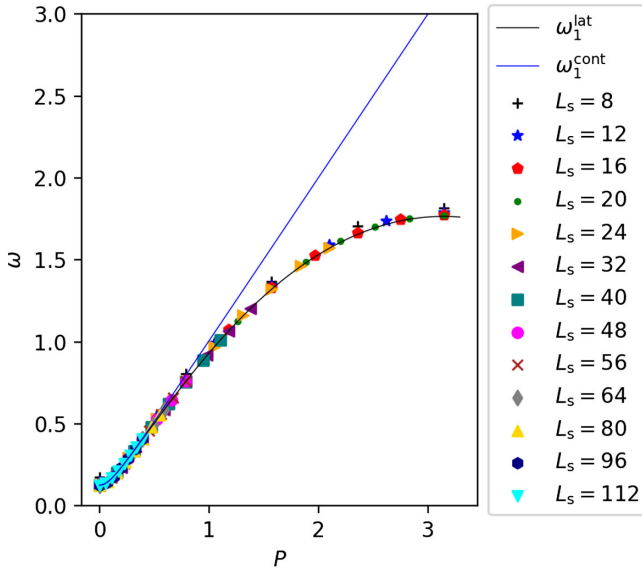


FIG. 10. One-particle state energy spectrum for $L_s = 8$ –112 computed with $L_t = 4$ and $\chi = 80$, together with the one-particle dispersion relation.

then the eigenstate $|a\rangle$ has total momentum P irrespective of p . To estimate $\langle \Omega | \hat{\mathcal{O}}_2(P, p) | a \rangle$, we coarse grain the impurity tensor network shown in Fig. 11. The numerical results of the matrix elements for $L_s = 64$ in total momentum $|d| = 0$ –5 sectors are listed in Table II. Similar to the $q = -1$ case, matrix elements with value $|\langle \Omega | \hat{\mathcal{O}}_2(P, p) | a \rangle| < 10^{-6}$ are treated as zero. Some elements of order $O(10^{-6})$ and $O(10^{-5})$ are considered as noise, as we observe that their values decrease for larger

bond dimension $\chi = 90$. For elements of order $O(10^{-4})$, some are treated as a signal when their values increase for larger χ , and as a noise when they decrease.

We observe that the energy in the $q = +1, P \neq 0$ sector exhibits a fourfold degeneracy,³ as also seen in Fig. 7. After identifying the momentum, it turns out that the fourfold degenerate states belong to two different absolute values of total momentum. This occurrence is related to the phase shift of the $(1+1)$ d Ising model, which will be explained Sec. III F 1. Furthermore, all states in Table II are two-particle states, identified by looking at their behavior over system size, and also by dispersion relation, as will be explained in Secs. III D and III F 4, respectively.

D. Number of particles

The simplest way to identify the number of particles contained in the eigenstates of a given sector is to examine the energy dependence on the system size. First, we analyze the $q = -1, P = 0$ sector. From Fig. 12, three distinct energy levels are observed. The lowest level corresponds to the one-particle state energy with $P = 0$, since it approaches m in large system size, where m is the rest mass given in Eq. (47). Meanwhile, the second and third levels are the three-particle states as they approach $3m$ as the system size increases.

Next, we analyze the energy spectrum in the $q = +1, P = 0$ sector across system size L_s . From Fig. 13, the networks with $L_t = 4$ and $L_t = 8$ yield almost the same energy level in the sector for each system size. The three energy levels in this sector shown by orange, green, and red markers, which are classified by looking at the shape of the corresponding wave function, see Sec. III E, are the two-particle state energy as they approach $\omega = 2m$ in the large system size.

On the other hand, the number of particles corresponding to the energy level shown by the violet marker in Fig. 13 cannot be clearly identified. Such states, in which the number of particles is not well identified, are found only in relatively small volumes (up to $L_s = 56$) in our calculations, therefore we cannot observe its behavior in the large volume. Furthermore, in Sec. III E, it will be shown that the wave function of this unidentified state is also different from the two-particle case with smaller amplitude. We expect that this is a four-particle state, although further investigation is required to confirm this interpretation. There are two possible directions for future work on the four-particle states. The first is to derive an appropriate four-particle quantization condition and compute the corresponding theoretical prediction using the relevant dispersion relation. The second one is to identify the four-particle states by analyzing their respective wave functions. This approach is based on the observation that the wave function of the

³For $L_s = 64$, the four-fold degenerate states are: $a = 9$ –12, 16–19, 21–24, 27–30, 38–41, 44–47.

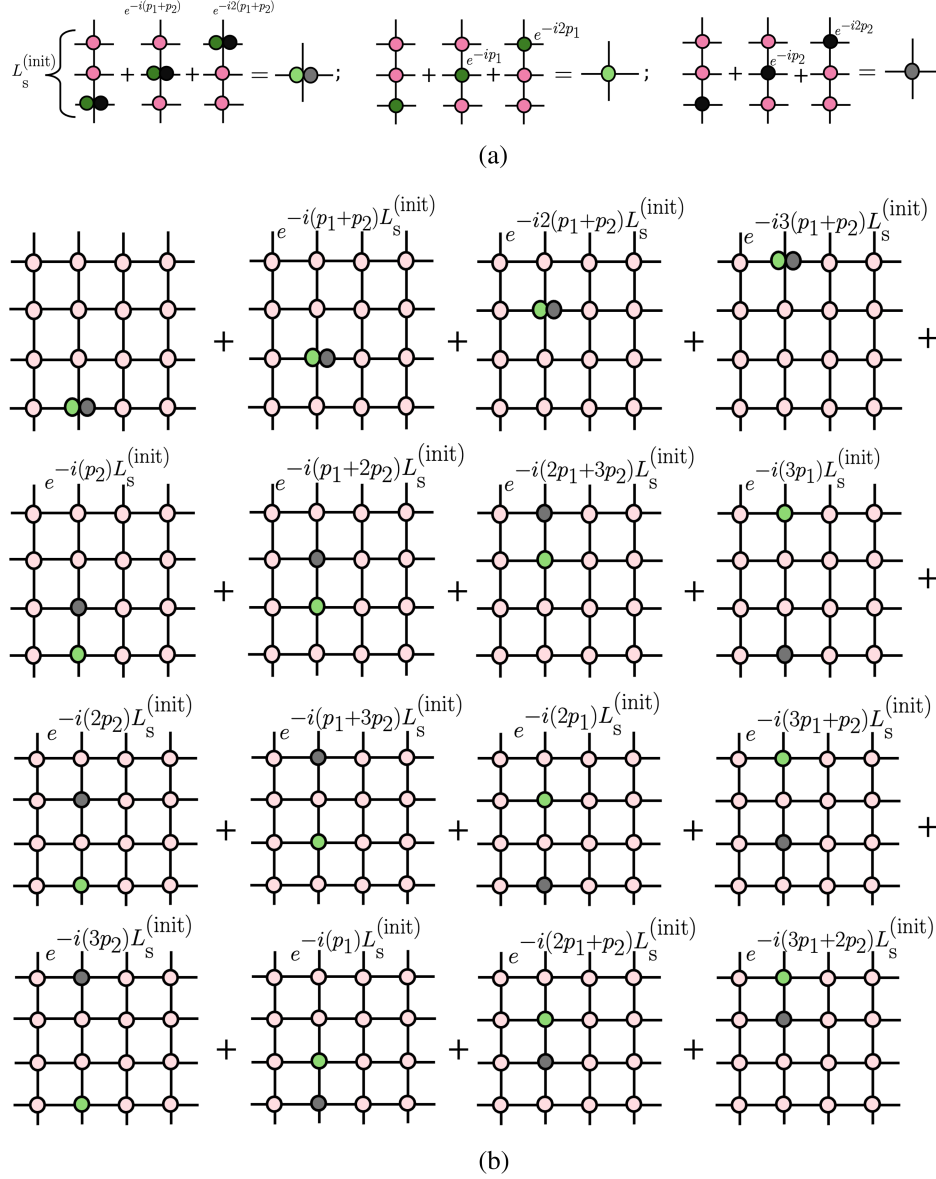


FIG. 11. (a) Pair of light green and gray circles represent the contracted initial impurity tensor network for two fields in momentum space. Meanwhile, the single light green (gray) circle denotes a single field in momentum space. These networks are constructed from bare pure tensors (dark pink circle) and some bare impurity tensors with proper momentum factors, namely: a pair of black and green circles, and single dark green (black) circle. Here, the initial network with $L_s^{(\text{init})} = 3$ is presented for readability. (b) The main impurity tensor network with total size $L_t \times L_s = 4 \times (L_s^{(\text{init})} \times 4)$ for the estimation of $\langle \Omega | \hat{O}_2(P, p) | a \rangle$.

possible four-particle states, as shown in Fig. 16(a), behaves differently from those of the two-particle states.

In addition, the energy spectrum in $q = +1$ for nonzero momentum sectors as function of system size is given in Fig. 14. In the figure, for this $d = 1-5$ sectors, one can clearly see that several energy levels approach $2m$ at large volumes, while this behavior is not evident for some other levels. Therefore, we cannot conclude from this figure alone that all the states shown here are two-particle states. However, as we will see later in Sec. III F 4, by comparing them with the dispersion relation for two-particle states, we find that all these states are indeed two-particle states.

E. Wave function

Wave function is also a useful quantity, as it allows direct extraction of important dynamical observables such as scattering phase shift. The procedure for computing the wave function with tensor network for the $q = -1$ sector has already been presented in [48], thus we focus here on the $q = +1$ sector.

The wave function of the energy eigenstate $|a\rangle$ in the $q = +1, P = 0$ sector can be computed by

$$\psi_a(x) = \langle \Omega | \hat{O}_2(x) | a \rangle. \quad (53)$$

TABLE II. Absolute value of matrix elements $|\langle \Omega | \hat{\mathcal{O}}_2(P, p) | a \rangle^{\text{[hotrg]}}|$ with $|P| = 0 - 10\pi/L_s$, for $L_s = 64$ computed using $\chi = 80$ and $L_t = 4$ for $|a\rangle$ in the $q = +1$ sector.

P	a						$ P $	$\omega_a^{\text{[hotrg]}}$
	0	$2\pi/L_s$	$4\pi/L_s$	$6\pi/L_s$	$8\pi/L_s$	$10\pi/L_s$		
6	0.206871	$<10^{-6}$	0.000008	$<10^{-6}$	0.000010	$<10^{-6}$	0	0.270811
9	$<10^{-6}$	0.092225	$<10^{-6}$	0.000012	$<10^{-6}$	0.000011	$2\pi/L_s$	0.329028
10	0.000019	$<10^{-6}$	0.045078	$<10^{-6}$	0.000001	$<10^{-6}$	$4\pi/L_s$	0.329029
11	$<10^{-6}$	$<10^{-6}$	0.045050	$<10^{-6}$	0.000010	$<10^{-6}$	$4\pi/L_s$	0.329038
12	$<10^{-6}$	0.092206	$<10^{-6}$	0.000028	$<10^{-6}$	0.000032	$2\pi/L_s$	0.329038
13	0.067467	$<10^{-6}$	0.000007	$<10^{-6}$	0.000005	$<10^{-6}$	0	0.38727
16	$<10^{-6}$	0.000002	$<10^{-6}$	0.053592	$<10^{-6}$	0.000027	$6\pi/L_s$	0.410097
17	$<10^{-6}$	0.000052	$<10^{-6}$	0.053624	$<10^{-6}$	0.000012	$6\pi/L_s$	0.410109
18	$<10^{-6}$	$<10^{-6}$	0.081047	$<10^{-6}$	0.000024	$<10^{-6}$	$4\pi/L_s$	0.410109
19	0.000069	$<10^{-6}$	0.081006	$<10^{-6}$	0.000058	$<10^{-6}$	$4\pi/L_s$	0.410111
21	0.000049	$<10^{-6}$	0.000040	$<10^{-6}$	0.008696	$<10^{-6}$	$8\pi/L_s$	0.468347
22	$<10^{-6}$	0.037856	$<10^{-6}$	0.000022	$<10^{-6}$	0.000002	$2\pi/L_s$	0.468362
23	$<10^{-6}$	$<10^{-6}$	0.000120	$<10^{-6}$	0.008682	$<10^{-6}$	$8\pi/L_s$	0.468414
24	$<10^{-6}$	0.037783	$<10^{-6}$	0.000105	$<10^{-6}$	0.000057	$2\pi/L_s$	0.468414
27	$<10^{-6}$	0.000014	$<10^{-6}$	0.079396	$<10^{-6}$	0.000171	$6\pi/L_s$	0.498128
28	0.000009	$<10^{-6}$	0.000075	$<10^{-6}$	0.059665	$<10^{-6}$	$8\pi/L_s$	0.498146
29	$<10^{-6}$	$<10^{-6}$	0.000077	$<10^{-6}$	0.059764	$<10^{-6}$	$8\pi/L_s$	0.498258
30	$<10^{-6}$	0.000172	$<10^{-6}$	0.079394	$<10^{-6}$	0.000118	$6\pi/L_s$	0.498259
35	0.045862	$<10^{-6}$	0.000492	$<10^{-6}$	0.000071	$<10^{-6}$	0	0.549592
38	0.000788	$<10^{-6}$	0.033879	$<10^{-6}$	0.000083	$<10^{-6}$	$4\pi/L_s$	0.556537
39	$<10^{-6}$	0.000050	$<10^{-6}$	0.000143	$<10^{-6}$	0.013012	$10\pi/L_s$	0.556644
40	$<10^{-6}$	0.000184	$<10^{-6}$	0.000152	$<10^{-6}$	0.012959	$10\pi/L_s$	0.556748
41	$<10^{-6}$	$<10^{-6}$	0.033987	$<10^{-6}$	0.000209	$<10^{-6}$	$4\pi/L_s$	0.556748
44	0.000192	$<10^{-6}$	0.000104	$<10^{-6}$	0.082079	$<10^{-6}$	$8\pi/L_s$	0.588224
45	$<10^{-6}$	0.000030	$<10^{-6}$	0.000231	$<10^{-6}$	0.066092	$10\pi/L_s$	0.588267
46	$<10^{-6}$	0.000053	$<10^{-6}$	0.000320	$<10^{-6}$	0.066321	$10\pi/L_s$	0.588615
47	$<10^{-6}$	$<10^{-6}$	0.000421	$<10^{-6}$	0.081789	$<10^{-6}$	$8\pi/L_s$	0.588615

The operator $\hat{\mathcal{O}}_2(x)$ is given by

$$\hat{\mathcal{O}}_2(x) = \frac{1}{L_s} \sum_{x'=0}^{L_s-1} \hat{s}_{x'} \hat{s}_{x'+x} \quad (54)$$

where $\hat{s}_x$ is the single spin field operator and x is the relative distance between the two operators [69]. From Eq. (53), we see that the wave function is obtained from matrix elements evaluated at each relative distance x . In Fig. 15, we show the impurity tensor network

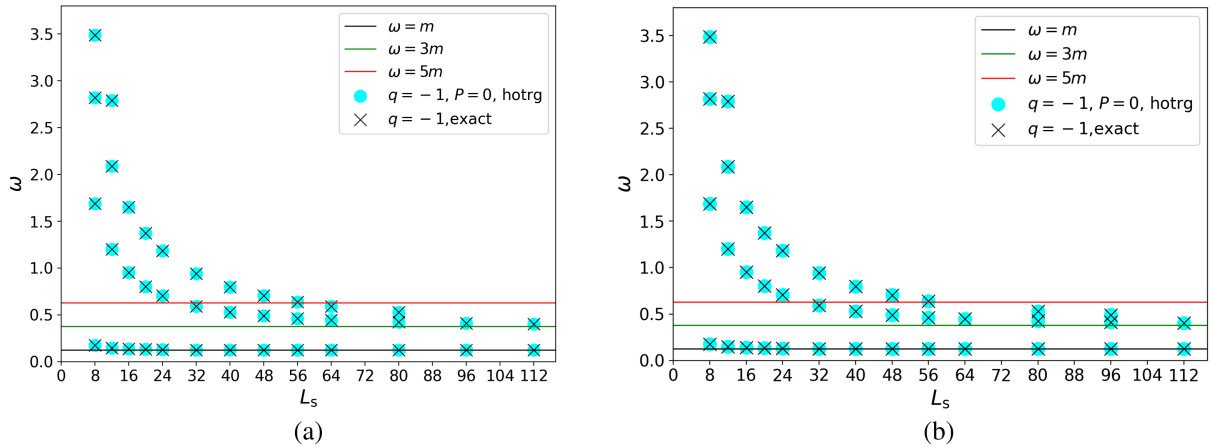


FIG. 12. Energy spectrum $\omega_a^{\text{[hotrg]}}$ from $q = -1$ and $P = 0$ sector over system size $L_s = 8-112$ computed using $\chi = 80$ with (a) $L_t = 4$, and (b) $L_t = 8$.

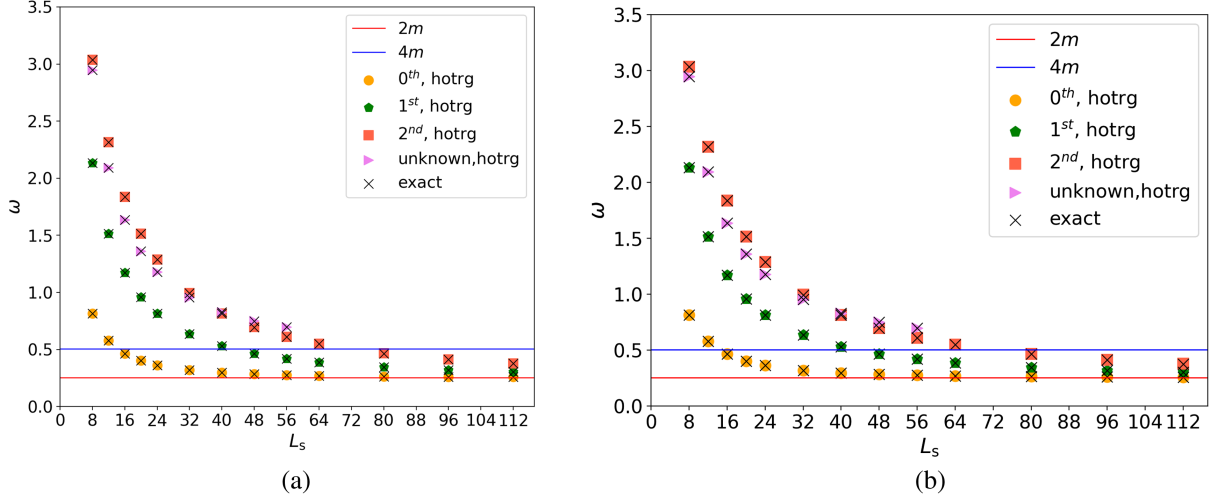


FIG. 13. Energy spectrum $\omega_a^{[\text{hotrg}]}$ from the $q = +1, P = 0$ sector over system size $L_s = 8-112$ computed using $\chi = 80$ with (a) $L_t = 4$ and (b) $L_t = 8$.

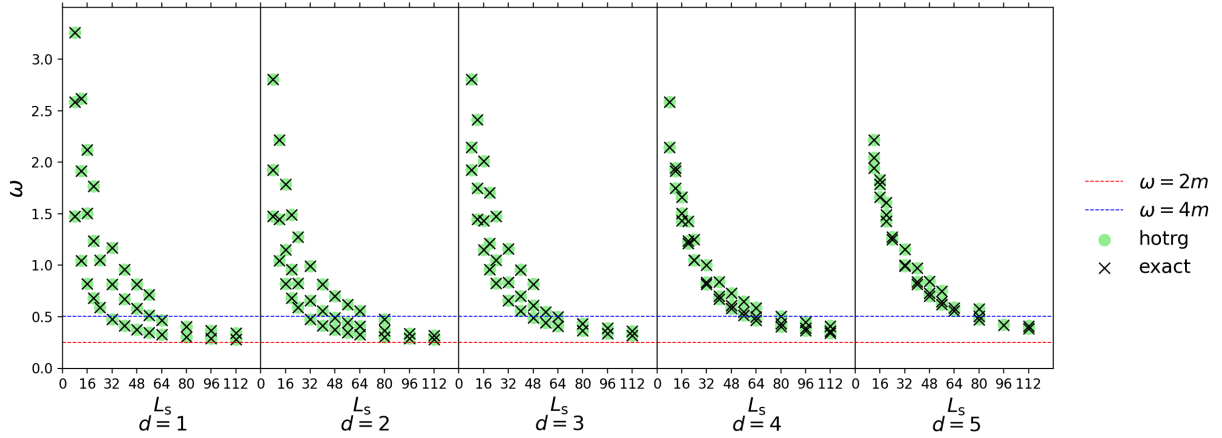


FIG. 14. Energy spectrum in the $q = +1$ and $d = 1-5$ sectors over system size L_s , computed with $L_t = 4$ and $\chi = 80$. The HOTRG data (green circles), represent the average energy of the degenerate states.

corresponding to the operator $\hat{O}_2(x)$ for $L_s = 4$ and $L_t = 4$. The extension to larger spatial sizes $L_s = 8-112$ and $L_t = 4, 8$ is straightforward. The computational cost of evaluating the wave function using HOTRG algorithm scales as $O(L_s^2 \chi^7)$. Owing to the symmetric property and PBC of the wave function,

$$\begin{aligned} \psi_a(L_s - x) &= \psi_a(-L_s + x) \\ &= \psi_a(x), \end{aligned} \quad (55)$$

which reduces the tensor network diagrams that need to be computed by half. We coarse grain the impurity tensor network shown in Fig. 15 and substitute the result into the Eq. (37) to obtain

$$\psi_a(x)^{[\text{hotrg}]} := \langle \Omega | \hat{O}_2(x) | a \rangle^{[\text{hotrg}]} \approx \langle \Omega | \hat{O}_2(x) | a \rangle. \quad (56)$$

The numerical results⁴ of the wave function⁵ $\psi_a(x)^{[\text{hotrg}]}$ computed with $L_t = 8$ and $L_s = 56$ coarse-grained with HOTRG using $\chi = 80$ are shown in Fig. 16(a). The wave functions, corresponding to $a = 6, 13, 37$, are the two-particle state wave function where the values at $x = 0$ are approximately zero, indicating that the two particles are

⁴We apply the sign normalization for the wave function so that $\psi_a(1)^{[\text{hotrg}]} > 1$ for all a and all L_s that is

$$\psi_a(x)^{[\text{hotrg}]} \leftarrow \psi_a(x)^{[\text{hotrg}]} \times \frac{\psi_a(1)^{[\text{hotrg}]}}{|\psi_a(1)^{[\text{hotrg]}|}. \quad (57)$$

⁵We show the wave function for $L_s = 56$, instead of $L_s = 64$, because $L_s = 56$ is the largest size where the unidentified state (possibly four-particle state) in the $q = +1, P = 0$ sector is obtained.

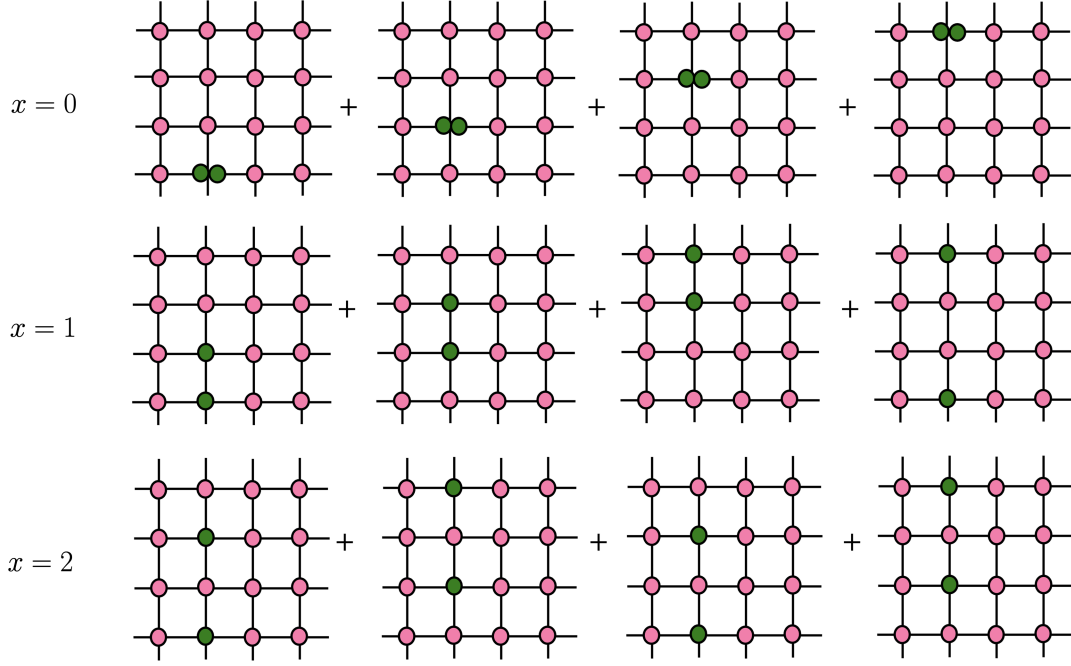


FIG. 15. Tensor network representation for the computation of two-particle state wave function $\psi_a(x)$ with system size $L_s = 4$ and $L_t = 4$. Due to PBC, it is sufficient to consider $x = 0, 1, 2$. Note that the green circles represent the impurity tensors.

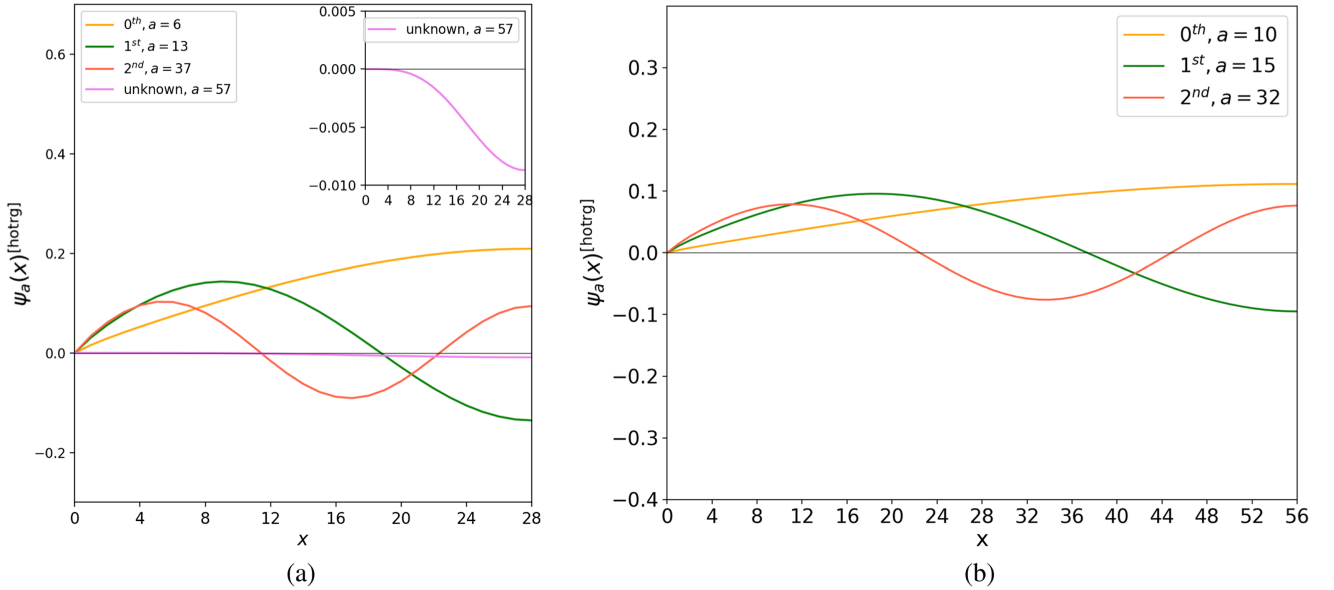


FIG. 16. (a) Wave function $\psi_a(x)$ in the $q = +1, P = 0$ sector computed with $L_t = 8$ and $\chi = 80$ for system size $L_s = 56$ corresponding to $a = 6, 13, 37, 57$. The inset shows an enlarged view of the wave function for $a = 57$. (b) The wave function for $L_s = 112$ computed with $\chi = 90$ and $L_t = 8$ corresponding to eigenstates $a = 10, 15, 32$.

never in contact. Here, the zeroth, first, and second wave functions are identified based on the number of nodes of $\psi_a(x)^{[\text{hotrg}]}$ within the region $0 < x \leq L_s/2$, where the zeroth wave function has no node, the first has one node, and so on. In contrast, the wave function corresponding to eigenstate number $a = 57$ exhibits qualitatively different behavior and has a relatively smaller amplitude. This behavior persists even at a larger bond dimension, $\chi = 90$. The similar wave

function, as $a = 57$ for $L_s = 56$, is also observed on other system sizes $L_s = 8\text{--}48$.

Furthermore, we show the wave function for $L_s = 112$ computed with $L_t = 8$ and $\chi = 90$ in Fig. 16(b). The wave function from larger system size is preferable for the subsequent analysis, that is the extraction of the phase shift from the wave function approach which, will be discussed in Secs. III F 2 and III F 3, and $L_s = 112$ is the

largest size accessible with $\chi = 90$, where at this size, two-particle state wave functions are obtained for the eigenstates $a = 10, 15, 32$.

F. Two-particle states analysis

Hereafter, we focus on the two-particle states and their dynamics. The scattering phase shift, as an important dynamical quantity, can be extracted from the finite volume energy spectrum as well as from the wave function of the two-particle states inside and outside interaction range, see Fig. 17. In the following, we show the procedure to determine the scattering phase shift using these three approaches.

1. Phase shift from the energy spectrum

The scattering phase shift can be extracted from the finite volume two-particle state energy spectrum in the center of mass (CM) frame ($P = 0$) as well as in the moving frame ($P \neq 0$). To this end, we compute the relative momentum p using two-particle lattice dispersion relation [74]

$$\omega_2^{(d)} = \cosh^{-1} \left(\cosh(m) + 1 - \cos \left(\frac{\pi}{L_s} d + p \right) \right) + \cosh^{-1} \left(\cosh(m) + 1 - \cos \left(\frac{\pi}{L_s} d - p \right) \right), \quad (58)$$

where the two-particle energy $\omega_a^{[\text{hotrg}]}$ is used as the input $\omega_2^{(d)}$. For $d \neq 0$, $\omega_2^{(d)}$ is taken to be the average of the degenerate energies. As a reminder, $d = 0, 1, \dots, L_s - 1$ is the integer related to the total momentum, as defined in Eq. (50). Note that $p = \gamma k$, where k is the relative momentum in the CM frame, with the Lorentz factor γ . When $d = 0$,

Lorentz factor is $\gamma = 1$, and the relative momentum satisfies $p = k$. In this case, the relative momentum p can be directly determined from Eq. (58). However, for $d \neq 0$, the equation must be solved numerically to obtain p , where in our analysis we employ the bisection method. Using the resulting relative momentum p , the phase shift can then be computed from Lüscher's formula [67,74,79] as follows

$$2\delta^{(d)} + pL_s + \pi d = 0 \pmod{2\pi}. \quad (59)$$

In Fig. 18, we show the scattering phase shift, $\delta^{(d)}$, extracted from the two-particle state energy for $d = 0 - 3$, computed using $L_t = 4, 8$ over k/m . For $d \neq 0$, the relative momentum p is transformed to the CM momentum k by first converting the moving frame energy to CM energy using [79]

$$\omega^{(\text{CM})} = \cosh^{-1} \left(\cosh(\omega^{(d)}) - 1 + \cos \frac{2\pi d}{L_s} \right), \quad (60)$$

with $\omega^{(d)}$ as an input. The resulting CM energy, $\omega^{(\text{CM})}$, is then substituted into Eq. (58) by setting $d = 0$ to determine k , which is used to compute k/m for the x axis in Fig. 18. The numerical results approximately agree with the theoretical Ising results [80]

$$\delta_{[\text{ising}]} = -\frac{\pi}{2}, \quad (61)$$

up to some errors. In general, the most accurate phase shift is obtained in the CM frame, i.e., for $d = 0$. We observe that the phase shift at small k/m , which corresponds to larger system size L_s , becomes less accurate due to the coarse-graining error. We also see that increasing cut-off bond dimension χ reduces the error of the phase shift, as expected.

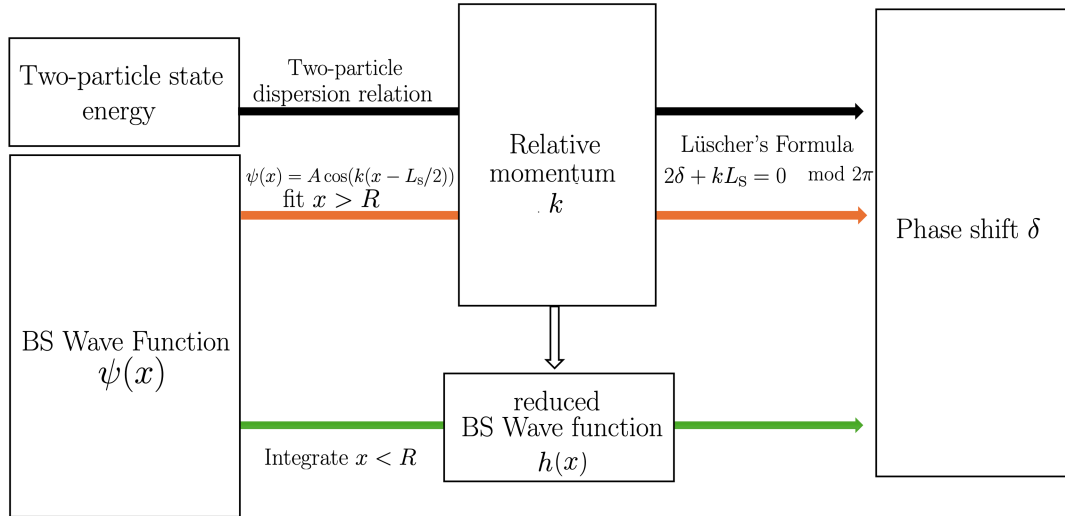


FIG. 17. Diagram of the two-particle state analysis performed in this work. The black arrow denotes the computation of the phase shift using only Lüscher's formula, the orange arrow indicates the flow of analysis using the BS wave function outside the interaction range R with the aid of Lüscher's formula, and the green arrow represents the flow using the BS wave function inside R , where information on relative momentum is required.

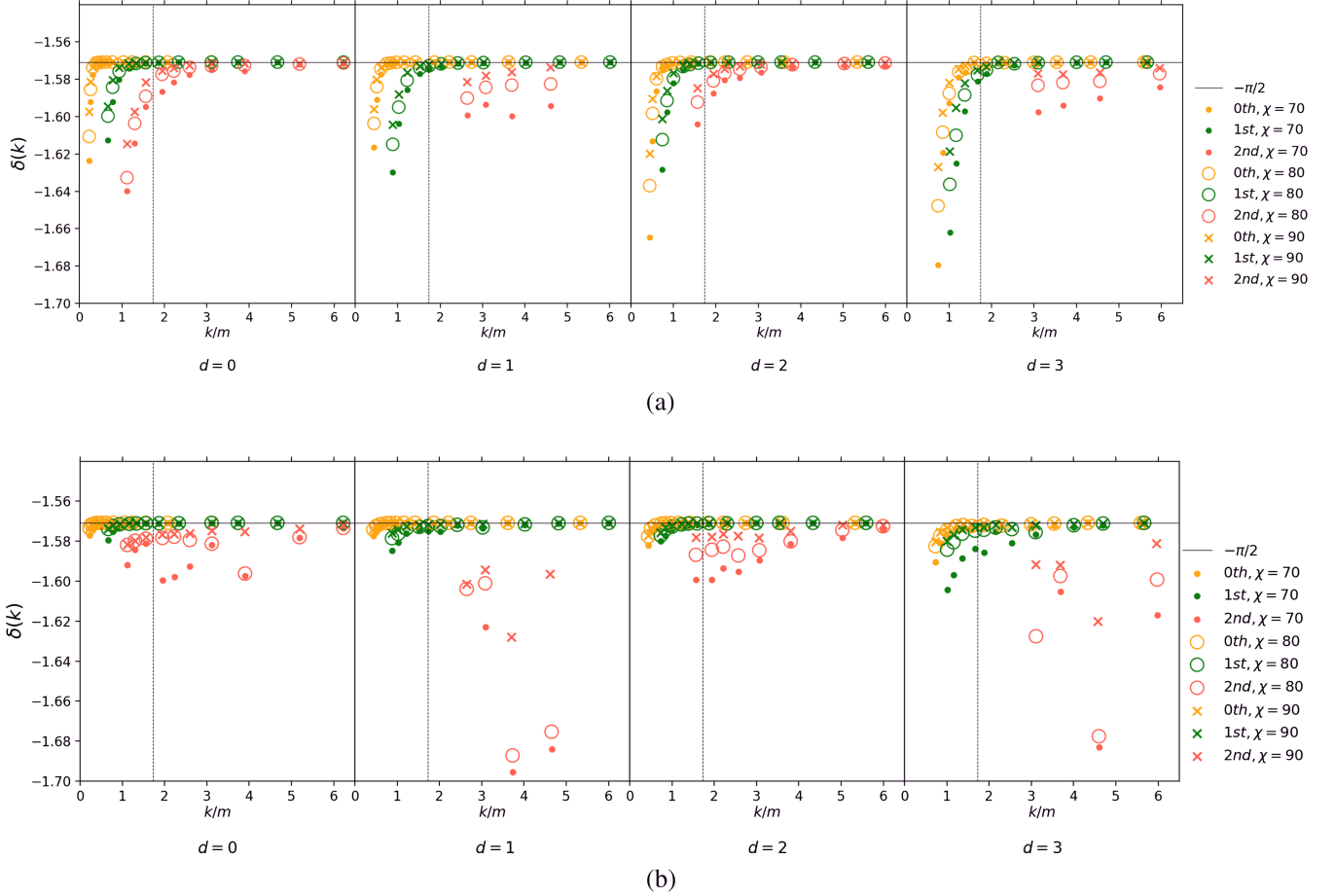


FIG. 18. Scattering phase shift of two-particle state on CM and moving frame, i.e. $d = 0, 1, 2, 3$ (from left to right) computed using $\chi = 80$ with (a) $L_t = 4$ and (b) $L_t = 8$. The vertical dashed line is the elastic limit $k/m = \sqrt{3}$.

2. Phase shift from the wave function outside interaction range

As previously mentioned, the phase shift can be extracted directly from the two-particle state wave function in the $P = 0$ sector, which is numerically computed by following the procedure described in Sec. III E. To extract the phase shift, we first compute the effective potential $V_{\text{eff}}(x)$ of the scattering

$$V_{\text{eff}}(x) = \frac{(\partial_x^2)^{\text{lat}} \psi(x)}{\psi(x)} + k_{\text{lat}}^2 \quad (62)$$

where $(\partial_x^2)^{\text{lat}} \psi(x) = \psi(x+1) - 2\psi(x) + \psi(x-1)$ with $\psi(x)^{[\text{hotrg}]}$ as input. Note that, the property $\psi(x) = \psi(-x)$ is used to compute the second derivative at $x = 0$ and $x = L_s/2$. Here,

$$k_{\text{lat}}^2 = 2(1 - \cos(k)) \quad (63)$$

where k is the relative momentum in CM, obtained from Eq. (58) with $d = 0$. The effective range R is defined as the range where V_{eff} is zero, that is

$$V_{\text{eff}}(x) = 0 \quad \text{for } x > R. \quad (64)$$

In Fig. 19, we present $V_{\text{eff}}(x)$ for the two-particle ground-state wave function of a system size $L_s = 112$, which was previously shown in Fig. 16(b). We observe that the effective potential $V_{\text{eff}}(x)$ diverges to infinity as $x \rightarrow 0$, indicating a strongly repulsive interaction between the two particles at the origin.⁶

For a system at temperature $T = 2.44$, we estimate the interaction range to be $R \approx 49$, since the lower error band of the effective potential, that is $V_{\text{eff}}(x) - \delta V_{\text{eff}}$, crosses zero

⁶Note that the numerical value of $\psi(0)$ is not exactly zero, but rather a very small number that may be either positive or negative. In our normalization, as mentioned in footnote 4, the wave function for small x can be expressed as $\psi(x) = c_1|x| + c_2x^2$ with $c_1 > 0$. The second derivative of $\psi(x)$ is then given by $\frac{d^2\psi(x)}{dx^2} = c_1\delta(x) + 2c_2$ where $\delta(x)$ is the delta function. Accordingly, the potential at $x = 0$ is given by

$$\lim_{x \rightarrow 0} V_{\text{eff}}(x) = \lim_{x \rightarrow 0} \frac{c_1\delta(x) + 2c_2}{c_1|x| + c_2x^2}, \quad (65)$$

which ensures $V_{\text{eff}}(x) \rightarrow +\infty$ for $x \rightarrow 0$.

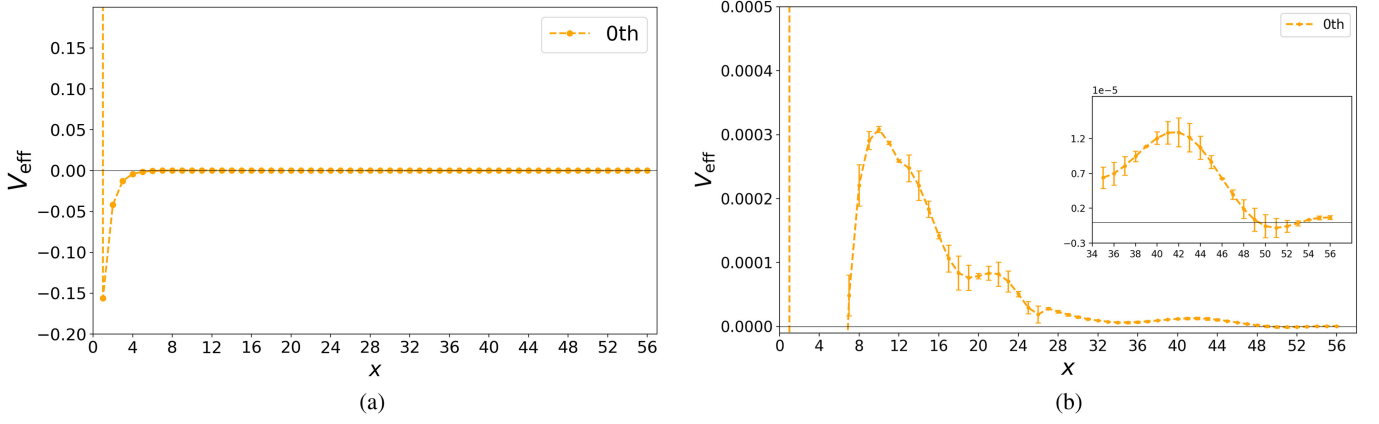


FIG. 19. (a) The effective potential from the two-particle ground state wave function for $L_s = 112$ and total momentum $P = 0$ computed using $L_t = 8$ and $\chi = 90$. (b) The same potential in a smaller scale together with the error band, which is given by $V_{\text{eff}} \pm \delta V_{\text{eff}}$, with $\delta V_{\text{eff}} = |V_{\text{eff}}(\chi = 90) - V_{\text{eff}}(\chi = 80)|$. The inset is the same data with scale in order 10^{-5} .

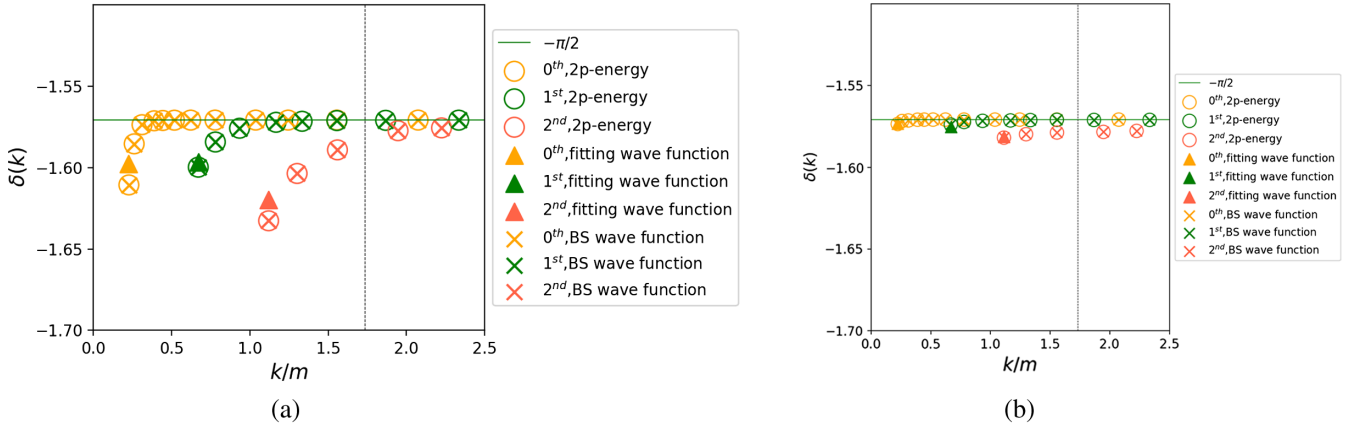


FIG. 20. Comparison of the phase shift in CM frame, computed at $\chi = 80$ using the finite volume energy, the fitting of the wave function outside the interaction range, and the Bethe-Salpeter wave function inside the interaction range for (a) $L_t = 4$ and (b) $L_t = 8$.

at $x = 49$, see Fig. 19. To estimate the systematic error, we compute effective potential using $\chi = 80$. Accordingly, the error δV_{eff} is simply given by $\delta V_{\text{eff}} = |V_{\text{eff}}(\chi = 90) - V_{\text{eff}}(\chi = 80)|$. Outside interaction range $x > R$, that is in the free region, the wave function is described as [69]

$$\begin{aligned} \psi(x)^{[\text{free}]} &= A \cos(kx + \delta) \\ &= A \cos(k(x - L_s/2)) \end{aligned} \quad (66)$$

where the second line is obtained with the aid of Lüscher's formula. Accordingly, A , a constant, and k , the relative momentum, are the fitting parameters. We fit the numerical wave function $\psi(x)^{[\text{hotrg}]}$, with the functional form $\psi(x)^{[\text{free}]}$ in the free region, $R < x \leq L_s/2$, extract k , and use the result to obtain the phase shift $\delta = -kL_s/2$. We apply this fitting procedure only for $L_s = 112$, since there is no free region for $L_s \leq 98$. The scattering phase shift obtained

using this approach is shown in Fig. 20. For $L_t = 8$, the results agree with those from finite volume energy of order $O(10^{-2})$, whereas for $L_t = 4$ larger discrepancies are observed, particularly for the ground state and second excited state. The reason is that, the wave functions from tensor network with large volume $L_s = 112$ and $L_t = 4$ are significantly affected by coarse-graining errors, leading to a large error in the fitting results.

3. Phase shift from the wave function inside interaction range

In contrast to the fitting procedure, which is evaluated outside interaction range, we show the extraction of phase shift from the inside of the interaction range by employing the Bethe-Salpeter (BS) wave function method [70–72]. For this purpose, first we recall the scattering amplitude for the $(1+1)\text{d}$ system in continuum space time

$$f(k) = \frac{e^{i\delta(k)}}{k} \sin \delta(k), \quad (67)$$

which corresponds to an amplitude $H(k)$, up to the overall phase factor, that is directly related to the BS wave function as follows

$$H(k) = -\frac{1}{2k^2} \int_{-\infty}^{\infty} dx h(x) g(x). \quad (68)$$

Here, $g(x)$ is a function satisfying $\partial_x^2 g(x) = -k^2 g(x)$, namely $g(x) = \cos(kx)$ or $g(x) = \sin(k|x|)$. Meanwhile, $h(x)$ is the reduced BS wave function

$$h(x) = (\partial_x^2 + k^2)\psi(x) \quad (69)$$

where $\psi(x)$ is the BS wave function. In the region $|x| > R$, $h(x) = 0$ corresponding to $V_{\text{eff}}(x) = 0$ in Eq. (64) and $\psi(x)$ is merely a free wave function that may be written as

$$\psi(x) = \begin{cases} A \cos(kx + \delta(k)) & x > R \\ A \cos(kx - \delta(k)) & x < -R \end{cases} \quad (70)$$

Using integration by parts and Eqs. (69), (68) can be written as

$$2k^2 H(k) = -[[\partial_x \psi(x)]g(x) - \psi(x)[\partial_x g(x)]]_{-R}^R. \quad (71)$$

For $g(x) = \cos(kx)$, the function $H(k)$ is denoted as $H_c(k)$. Substituting $g(x) = \cos(kx)$ and Eq. (70) into Eq. (71), we obtain $H_c(k) = \sin(\delta(k))/k$. Similarly, for $g(x) = \sin(k|x|)$, we denote $H(k)$ as $H_s(k)$, which is given by $H_s(k) = \cos(\delta(k))/k$. Consequently, the ratio of H_s/H_c determines the scattering phase shift $\delta(k) = \cot^{-1}(H_s(k)/H_c(k))$.

For the computation, the lattice counterparts of the amplitude, H_s^{lat} and H_c^{lat} , are employed. For a given momentum, they are given by

$$2k_{\text{lat}}^2 H_c^{\text{lat}}(k; x) = - \sum_{z=0}^x n(z) h^{\text{lat}}(k; z) \cos(kz) \quad (72)$$

$$2k_{\text{lat}}^2 H_s^{\text{lat}}(k; x) = - \sum_{z=0}^x n(z) h^{\text{lat}}(k; z) \sin(k|z|) \quad (73)$$

where $n(0) = n(L_s/2) = 1$, $n(z) = 2$ for other z , and $x = 1, 2, \dots, L_s/2$. Here, $h^{\text{lat}}(k; z)$ is the lattice version of the reduced BS wave function in Eq. (69) that is given by

$$h^{\text{lat}}(k; z) = \psi(z+1) - 2\psi(z) + \psi(z-1) + k_{\text{lat}}^2 \psi(z). \quad (74)$$

Using Eqs. (72)–(74), with $\psi(x)^{\text{[hotrg]}}$ as the input, the effective phase shift as a function of x is extracted from

$$\delta(k; x) = \cot^{-1} \left(\frac{H_s^{\text{lat}}(k; x)}{H_c^{\text{lat}}(k; x)} \right) \quad \text{for } 0 \leq x \leq L_s/2. \quad (75)$$

In Fig. 21, we show $\delta(k; x)$ from the wave function data for system size $L_s = 112$ and $L_t = 4, 8$ with cutoff $\chi = 80$. This figure shows that the phase shift deviates from $-\pi/2$ for $x < R$ while it approaches $-\pi/2$ for $x > R$. Comparing Figs. 21(a) and 21(b), we find that the data from $L_t = 8$ gives $\delta(k; x)$ closer to the theoretical value $-\pi/2$ for large x compared to $L_t = 4$.

For every $L_s = 8\text{--}112$, we compute $\delta(k; x)$ using Eq. (75). We select the value at $x = L_s/2$, that is $\delta(k; L_s/2)$, and plot them in Fig. 20. We observe that the result from Lüscher's method and from the reduced BS wave function agree up to double precision for all L_s and for both $L_t = 4, 8$. This agreement can be understood from the fact that Eq. (75) turns into Lüscher's formula for $x = L_s/2$, as discussed in the Appendix.

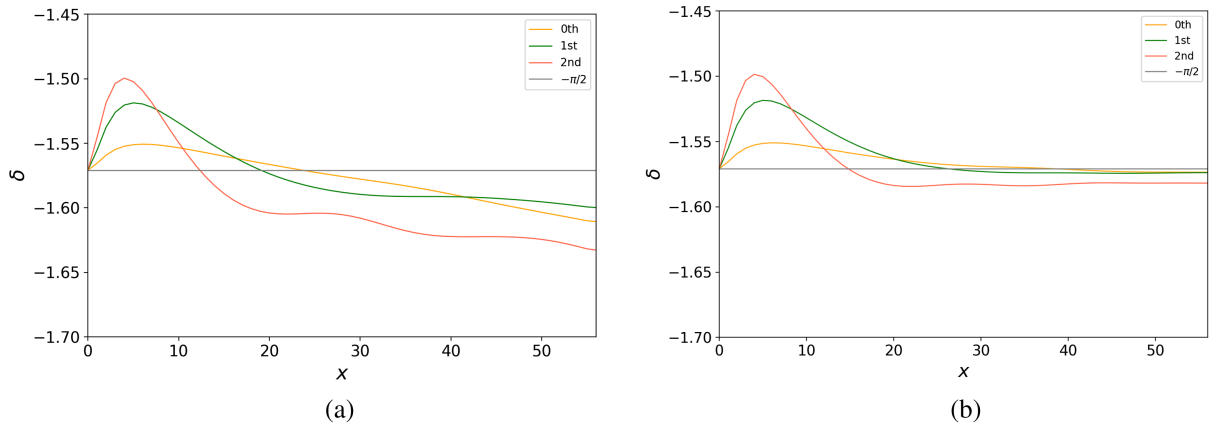


FIG. 21. Effective phase shift $\delta(k; x)$ computed by using Eq. (75) over $0 \leq x \leq L_s/2$ at system size $L_s = 112$ computed with $\chi = 80$ and (a) $L_t = 4$, (b) $L_t = 8$.

TABLE III. Momentum of p_1 , p_2 for two-particle state in $|d| = 1-5$ sector for fourfold degenerate states.

P	$\frac{2\pi}{L_s}$	$\frac{-2\pi}{L_s}$	$\frac{4\pi}{L_s}$	$\frac{-4\pi}{L_s}$	$\frac{4\pi}{L_s}$	$\frac{-4\pi}{L_s}$	$\frac{6\pi}{L_s}$	$\frac{-6\pi}{L_s}$	$\frac{2\pi}{L_s}$	$\frac{-2\pi}{L_s}$	$\frac{8\pi}{L_s}$	$\frac{-8\pi}{L_s}$
d	+1	-1	+2	-2	+2	-2	+3	-3	+1	-1	+4	-4
n	1	0	1	-1	2	0	2	-1	2	1	2	-2
p_1	$\frac{3\pi}{L_s}$	$\frac{\pi}{L_s}$	$\frac{3\pi}{L_s}$	$\frac{-\pi}{L_s}$	$\frac{5\pi}{L_s}$	$\frac{\pi}{L_s}$	$\frac{5\pi}{L_s}$	$\frac{-\pi}{L_s}$	$\frac{5\pi}{L_s}$	$\frac{3\pi}{L_s}$	$\frac{5\pi}{L_s}$	$\frac{-3\pi}{L_s}$
p_2	$\frac{-\pi}{L_s}$	$\frac{-3\pi}{L_s}$	$\frac{\pi}{L_s}$	$\frac{-3\pi}{L_s}$	$\frac{-\pi}{L_s}$	$\frac{-5\pi}{L_s}$	$\frac{\pi}{L_s}$	$\frac{-5\pi}{L_s}$	$\frac{-3\pi}{L_s}$	$\frac{-5\pi}{L_s}$	$\frac{3\pi}{L_s}$	$\frac{-5\pi}{L_s}$
P	$\frac{6\pi}{L_s}$	$\frac{-6\pi}{L_s}$	$\frac{8\pi}{L_s}$	$\frac{-8\pi}{L_s}$	$\frac{4\pi}{L_s}$	$\frac{-4\pi}{L_s}$	$\frac{10\pi}{L_s}$	$\frac{-10\pi}{L_s}$	$\frac{8\pi}{L_s}$	$\frac{-8\pi}{L_s}$	$\frac{10\pi}{L_s}$	$\frac{-10\pi}{L_s}$
d	+3	-3	+4	-4	+2	-2	+5	-5	+4	-4	+5	-5
n	3	0	3	-1	3	1	3	-2	4	0	4	-1
p_1	$\frac{7\pi}{L_s}$	$\frac{\pi}{L_s}$	$\frac{7\pi}{L_s}$	$\frac{-\pi}{L_s}$	$\frac{7\pi}{L_s}$	$\frac{3\pi}{L_s}$	$\frac{7\pi}{L_s}$	$\frac{-3\pi}{L_s}$	$\frac{9\pi}{L_s}$	$\frac{\pi}{L_s}$	$\frac{9\pi}{L_s}$	$\frac{-\pi}{L_s}$
p_2	$\frac{-\pi}{L_s}$	$\frac{-7\pi}{L_s}$	$\frac{\pi}{L_s}$	$\frac{-7\pi}{L_s}$	$\frac{-3\pi}{L_s}$	$\frac{-7\pi}{L_s}$	$\frac{3\pi}{L_s}$	$\frac{-7\pi}{L_s}$	$\frac{-\pi}{L_s}$	$\frac{-9\pi}{L_s}$	$\frac{\pi}{L_s}$	$\frac{-9\pi}{L_s}$

4. Degeneracy of two-particle states

From Secs. III F, III F 2, and III F 3, we observe that the two-particle scattering phase shift of the $(1+1)$ -dimensional Ising model is always $-\pi/2$ for any k/m , both inside and outside the elastic region $0 \leq k/m < \sqrt{3}$. This feature leads to fourfold degeneracies in the energy spectrum in the moving frame as shown in Sec. III D, which can be understood as follows. First, inserting Eq. (61) into Eq. (59) makes the allowed relative momentum

$$p = \frac{\pi}{L_s}(1 - d + 2n), \quad n \in \mathbb{Z}. \quad (76)$$

Using Eq. (51) and $P = p_1 + p_2$, the p_1 and p_2 are given by

$$p_1 = \frac{(2n+1)\pi}{L_s}, \quad p_2 = \frac{(2d-2n-1)\pi}{L_s}. \quad (77)$$

Using Eq. (77) and assuming $p_1 > p_2$ ($p > 0$), we find that there are four combinations of momenta (p_1, p_2) , as listed in Table III for $|d| = 1-5$, that yield the same energy when substituted into the following two-particle dispersion relation:

$$\omega_2^{\text{lat}} = \sum_{i=1}^2 \cosh^{-1}(\cosh m + 1 - \cos p_i). \quad (78)$$

Note that, this expression is the same as Eq. (58), with $p_1 = \frac{\pi d}{L_s} + p$ and $p_2 = \frac{\pi d}{L_s} - p$. It can be verified that the information of the total momenta P for fourfold degenerate energy in Table III are consistent with those previously listed in Table II for $L_s = 64$.

In addition, from Fig. 22 we observe that the numerical two-particle state energy levels previously presented in Fig. 14 are consistent with those obtained from the dispersion relation given by Eq. (78). This provides further evidence for the identification of the total momentum and the number of particles for the eigenstates in the $q = +1$ sector, as discussed in Secs. III C and III D.

G. Three-particle states analysis

1. Three-particle states energy momentum relation

In Sec. III C, we mentioned that some of the eigenstates in the $q = -1$ sector for $L_s = 64$, namely $a = 20, 48, 31-34, 36, 37, 49-52$, and $53, 54$, do not follow the one-particle dispersion relation. By applying the same procedure for other system sizes, such states can also be obtained. For the $P = 0$ case, the eigenstates with $a = 20, 48$ for $L_s = 64$

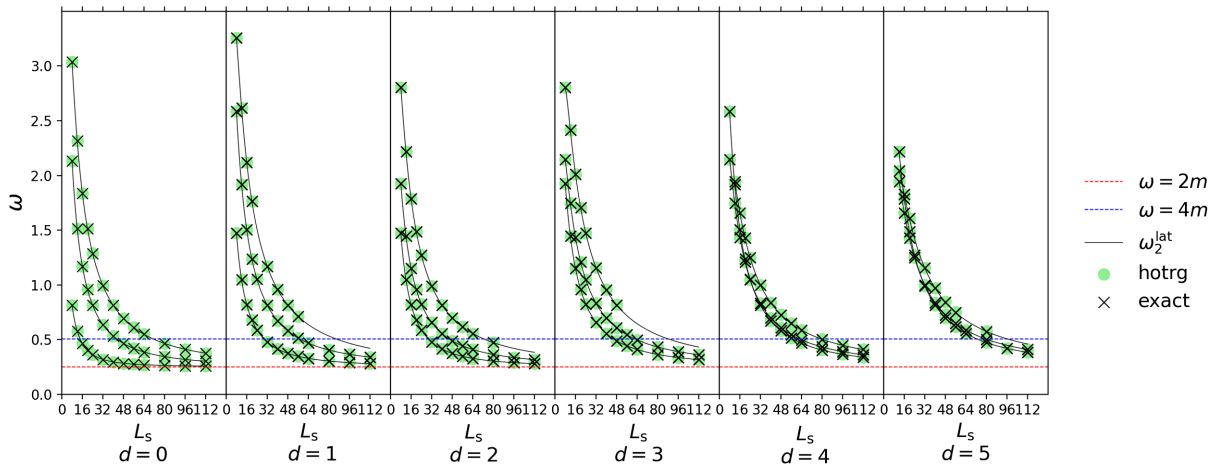


FIG. 22. Finite volume energy of two-particle states in the CM and moving frames, for $d = 0-5$ computed with $L_t = 4$ and $\chi = 80$, together with the two-particle states dispersion relation in Eq. (78). In the $d \neq 0$ sectors, the HOTRG data (green circles) represent the average of the degenerate energies.

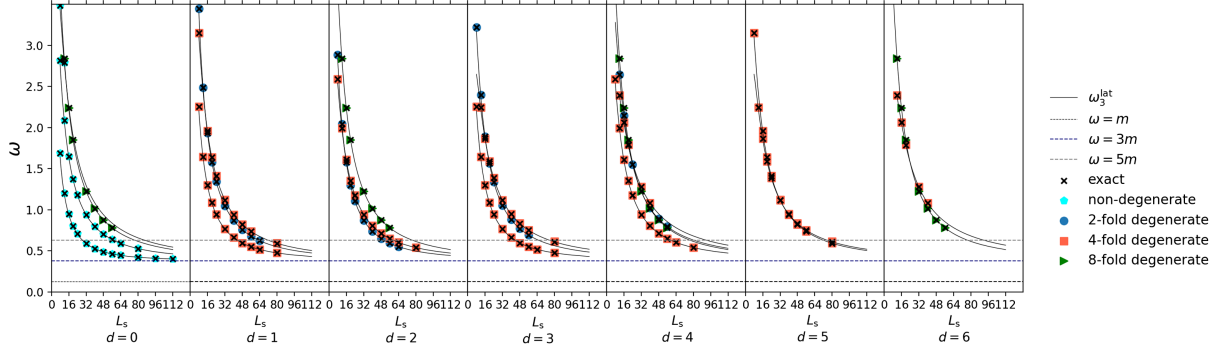


FIG. 23. Finite-volume energy of three-particle states for $d = 0-6$ computed with $L_t = 4$ and $\chi = 80$, together with the three-particle dispersion relation in Eq. (79). For degenerate states, the HOTRG data shown in the figure represent the average of the corresponding two-, four-, and eightfold degenerate energy.

have been identified as three-particle states in Sec. III D, as their energy approach $3m$ at large system sizes; see Fig. 12. The same argument can be applied for the $P \neq 0$ sector. However, some of the states cannot be clearly confirmed to belong to the three-particle sector solely on the energy dependence of system size, as they are only obtained up to relatively smaller sizes; see Fig. 23.

Therefore, to verify the number of particles, we compute the three-particle lattice dispersion relation [74]

$$\omega_3^{\text{lat}} = \sum_{i=1}^3 \cosh^{-1}(\cosh(m) + 1 - \cos(p_i)) \quad (79)$$

where p_i for $i = 1, 2, 3$ is the momentum. The momenta p_1, p_2 can be computed from the quantization condition derived by assuming that only pairwise interactions occur, that is [74]

$$2(\delta(-q_{31}) + \delta(q_{12})) - PL_s + p_1 L_s = 2\pi j_1, \quad (80)$$

$$2(\delta(-q_{23}) + \delta(q_{12})) + PL_s - p_2 L_s = 2\pi j_2, \quad (81)$$

where $j_1, j_2 \in \mathbb{Z}$, while p_3 is constrained by $p_3 = P - p_1 - p_2$. Here, δ is the two-particle state phase shift, which depends on the relative momentum of two interacting particles $q_{ij} = \frac{1}{2}(p_i - p_j)$, namely: $q_{12} = (p_1 - p_2)/2$, $q_{23} = (p_2 - p_3)/2$ and $q_{31} = (p_3 - p_1)/2$. Inserting the theoretical prediction for the two-particle scattering phase shift in Eq. (61), we solve Eqs. (80) and (81) to obtain p_1, p_2, p_3 as follows

$$\begin{aligned} p_1 &= \frac{2\pi}{L_s}(d + j_1), & p_2 &= \frac{2\pi}{L_s}(d - j_2), \\ p_3 &= \frac{2\pi}{L_s}(j_2 - j_1 - d), \end{aligned} \quad (82)$$

where d is the integer related to the total momentum $P = 2\pi d/L_s$. For a given d , (j_1, j_2) is chosen such that $q_{12} > 0$, and $q_{23} < 0, q_{31} < 0$ are satisfied. By substituting the resulting values p_1, p_2, p_3 as listed in Tables IV–VI, into

the dispersion relation in Eq. (79), we obtain predictions for the three-particle state energy. In fact, the theoretical predictions agree with the numerical data well. Following this procedure, we show in Fig. 23 that the remaining unidentified eigenstates in $q = -1$ sector, obtained by our scheme for $d = 0-6$, are indeed three-particle states.

2. Degeneracy of three-particle states

The degeneracy structure in three-particle sector of $(1+1)d$ Ising model is more varied than the one- or two-particle state. For $P = 0$, the three-particle states are nondegenerate. In contrast, for $P \neq 0$, as a consequence of the value of the phase shift in Eq. (61) being unchanged for any kinematics region, the spectrum exhibits not only twofold degeneracies, as in the one-particle state case, but also four-, and eightfold degeneracies as shown in Fig. 23. In Tables IV–VI, we categorize all possible combinations of momenta p_1, p_2, p_3 that yield the same energy in Eq. (79) into a separate column. In this case, Table IV shows the momenta for non- and twofold degeneracies, Table V shows the momenta for fourfold degeneracy, and Table VI shows the eightfold degeneracy.

With this explanation in mind, one can revisit Table I for $L_s = 64$, and identify nondegenerate, twofold degenerate, and fourfold degenerate three-particle states. The non-degenerate states correspond to $a = 20, 48$, the twofold degenerate states to $a = 36, 37, 53, 54$, and the fourfold

TABLE IV. Momentum of p_1, p_2, p_3 for the three-particle state in $|d| = 0-4$ sectors for non- and twofold degenerate states.

P	0	0	0	$\frac{2\pi}{L_s}$	$-\frac{2\pi}{L_s}$	$\frac{4\pi}{L_s}$	$-\frac{4\pi}{L_s}$	$\frac{6\pi}{L_s}$	$-\frac{6\pi}{L_s}$	$\frac{8\pi}{L_s}$	$-\frac{8\pi}{L_s}$
d	0	0	0	+1	-1	+2	-2	+3	-3	+4	-4
p_1	$\frac{2\pi}{L_s}$	$\frac{4\pi}{L_s}$	$\frac{6\pi}{L_s}$	$\frac{4\pi}{L_s}$	$\frac{4\pi}{L_s}$	$\frac{4\pi}{L_s}$	$\frac{2\pi}{L_s}$	$\frac{6\pi}{L_s}$	$\frac{2\pi}{L_s}$	$\frac{8\pi}{L_s}$	$\frac{2\pi}{L_s}$
p_2	$-\frac{2\pi}{L_s}$	$-\frac{4\pi}{L_s}$	$-\frac{6\pi}{L_s}$	$-\frac{4\pi}{L_s}$	$-\frac{4\pi}{L_s}$	$-\frac{2\pi}{L_s}$	$-\frac{4\pi}{L_s}$	$-\frac{2\pi}{L_s}$	$-\frac{6\pi}{L_s}$	$-\frac{2\pi}{L_s}$	$-\frac{8\pi}{L_s}$
p_3	0	0	0	$\frac{2\pi}{L_s}$	$-\frac{2\pi}{L_s}$	$\frac{2\pi}{L_s}$	$-\frac{2\pi}{L_s}$	$\frac{2\pi}{L_s}$	$-\frac{2\pi}{L_s}$	$\frac{2\pi}{L_s}$	$-\frac{2\pi}{L_s}$

TABLE V. Momentum of p_1, p_2, p_3 for three-particle state in $|d| = 1-6$ sectors for fourfold degenerate states.

P	$\frac{2\pi}{L_s}$	$-\frac{2\pi}{L_s}$	$\frac{6\pi}{L_s}$	$-\frac{6\pi}{L_s}$	$\frac{4\pi}{L_s}$	$-\frac{4\pi}{L_s}$	$\frac{8\pi}{L_s}$	$-\frac{8\pi}{L_s}$	$\frac{6\pi}{L_s}$	$-\frac{6\pi}{L_s}$	$\frac{10\pi}{L_s}$	$-\frac{10\pi}{L_s}$	$\frac{8\pi}{L_s}$	$-\frac{8\pi}{L_s}$	$\frac{12\pi}{L_s}$	$-\frac{12\pi}{L_s}$	$\frac{2\pi}{L_s}$	$-\frac{2\pi}{L_s}$	$\frac{10\pi}{L_s}$	$-\frac{10\pi}{L_s}$
d	+1	-1	+3	-3	+2	-2	+4	-4	+3	-3	+5	-5	+4	-4	+6	-6	+1	-1	+5	-5
p_1	$\frac{4\pi}{L_s}$	$\frac{2\pi}{L_s}$	$\frac{4\pi}{L_s}$	0	$\frac{6\pi}{L_s}$	$\frac{2\pi}{L_s}$	$\frac{6\pi}{L_s}$	0	$\frac{8\pi}{L_s}$	$\frac{2\pi}{L_s}$	$\frac{8\pi}{L_s}$	0	$\frac{10\pi}{L_s}$	$\frac{2\pi}{L_s}$	$\frac{10\pi}{L_s}$	0	$\frac{6\pi}{L_s}$	$\frac{4\pi}{L_s}$	$\frac{6\pi}{L_s}$	0
p_2	$-\frac{2\pi}{L_s}$	$-\frac{4\pi}{L_s}$	0	$-\frac{4\pi}{L_s}$	$-\frac{2\pi}{L_s}$	$-\frac{6\pi}{L_s}$	0	$-\frac{6\pi}{L_s}$	$-\frac{2\pi}{L_s}$	$-\frac{8\pi}{L_s}$	0	$-\frac{8\pi}{L_s}$	$-\frac{2\pi}{L_s}$	$-\frac{10\pi}{L_s}$	0	$-\frac{10\pi}{L_s}$	$-\frac{4\pi}{L_s}$	$-\frac{6\pi}{L_s}$	0	$-\frac{6\pi}{L_s}$
p_3	0	0	$\frac{2\pi}{L_s}$	$-\frac{2\pi}{L_s}$	0	0	$\frac{2\pi}{L_s}$	$-\frac{2\pi}{L_s}$	0	0	$\frac{2\pi}{L_s}$	$-\frac{2\pi}{L_s}$	0	0	$\frac{2\pi}{L_s}$	$-\frac{2\pi}{L_s}$	0	0	$\frac{4\pi}{L_s}$	$-\frac{4\pi}{L_s}$

TABLE VI. Momentum of p_1, p_2, p_3 for three-particle state in $|d| = 0, 2, 4, 6$ sectors for eightfold degenerate states.

P	0	0	$\frac{4\pi}{L_s}$	$-\frac{4\pi}{L_s}$	$\frac{8\pi}{L_s}$	$-\frac{8\pi}{L_s}$	$\frac{12\pi}{L_s}$	$-\frac{12\pi}{L_s}$
d	0	0	+2	-2	+4	-4	+6	-6
p_1	$\frac{4\pi}{L_s}$	$\frac{6\pi}{L_s}$	$\frac{6\pi}{L_s}$	$\frac{4\pi}{L_s}$	$\frac{6\pi}{L_s}$	$\frac{2\pi}{L_s}$	$\frac{6\pi}{L_s}$	$-\frac{2\pi}{L_s}$
p_2	$-\frac{6\pi}{L_s}$	$-\frac{4\pi}{L_s}$	$-\frac{4\pi}{L_s}$	$-\frac{6\pi}{L_s}$	$-\frac{2\pi}{L_s}$	$-\frac{6\pi}{L_s}$	$\frac{2\pi}{L_s}$	$-\frac{6\pi}{L_s}$
p_3	$\frac{2\pi}{L_s}$	$-\frac{2\pi}{L_s}$	$\frac{2\pi}{L_s}$	$-\frac{2\pi}{L_s}$	$\frac{4\pi}{L_s}$	$-\frac{4\pi}{L_s}$	$\frac{4\pi}{L_s}$	$-\frac{4\pi}{L_s}$

degenerate states to $a = 31-34$, $a = 49-52$. However, eightfold degenerate states are not listed in the table, as for $L_s = 64$ they likely appear in eigenstates with $a > 57$, which cannot be reliably extracted with $L_t = 4$ and $\chi = 80$. In our calculation, with cutoff $\chi = 80$, the eightfold degenerate states are only obtained for system sizes $L_s = 8-56$ as shown in Fig. 23.

IV. SUMMARY

In this paper, we have investigated the multiparticle states by applying the spectroscopy scheme introduced in [48] with the updated coarse-graining strategy and demonstrated it to the $(1+1)$ d Ising model. We find that tensor networks with $L_t = 4, 8$ yield energy spectra with smaller errors than other choices of L_t . Consequently, the higher excited state energy than those reported in [48], as well as their corresponding quantum numbers $q = \pm 1$ can be reliably determined with the relative error in order $O(10^{-3})$. We further confirmed that the errors for $L_t = 4, 8$ decrease with increasing the bond dimension.

Next, we identified the total momentum of the eigenstates in the $q = -1$ and $q = +1$ sectors for $L_s = 8-112$ using the matrix elements of the appropriate operators. From the $q = -1$ sector, we observed not only one-particle states but also three-particle states with $|P| = 0-12\pi/L_s$. The classification of one- and three-particle states for each momentum is done by observing the behavior of the energy as a function of system size, as well as from their respective dispersion relations. Similarly, in the $q = +1$ sector, the two-particle states with $|P| = 0-10\pi/L_s$ are also clearly identified.

In addition, we successfully computed the wave function of the two-particle state with $P = 0$, from the ground to the second excited state, by employing the impurity tensor network method. From the ground state wave function, the effective potential is computed, and we use it to estimate the interaction range R , where for $T = 2.44$ it is approximately $R \approx 49$. Furthermore, we extracted the scattering phase shift of the two-particle state using three approaches: the finite volume energy approach in both the CM and moving frames using Lüscher's formula, fitting the two-particle wave function outside the interaction range, and the BS wave function method from inside interaction range. The results obtained from all three methods are consistent with each other as well as with the theoretical prediction up to the error. From this calculation, we confirmed that the phase shift of the $(1+1)$ d Ising model is always given by $\delta = -\pi/2$ for any relative momentum. As a consequence, in the two-particle state sector, some states with different total momenta become fourfold degenerate.

Lastly, in the three-particle sector, the numerical results agree with the theoretical prediction for the finite volume three-particle energy, which is computed under the assumption that no three-body interaction occurs. In this sector, the energy are also degenerated where the degeneracies are more varied and include: twofold degeneracy, as well as fourfold and eightfold degeneracies.

For future work, we will continue to the investigation of four-particle states, and the application of the scheme to other quantum field theories.

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DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

APPENDIX: LÜSCHER'S FORMULA FROM BETHE SALPETER WAVE FUNCTION

In this Section, we will derive the Lüscher's formula from the BS wave function. For this purpose, we compute $H_c^{\text{lat}}(k; L_s/2)$, and $H_s^{\text{lat}}(k; L_s/2)$ in Eqs. (72) and (73) for $x = L_s/2$, that is

$$2k_{\text{lat}}^2 H_c^{\text{lat}}(k; L_s/2) = - \sum_{z=0}^{L_s/2} n(z) h(k; z) \cos(kz), \quad (\text{A1})$$

$$2k_{\text{lat}}^2 H_s^{\text{lat}}(k; L_s/2) = - \sum_{z=0}^{L_s/2} n(z) h(k; z) \sin(k|z|), \quad (\text{A2})$$

where $n(z) = 1$ for $z = 0, L_s/2$ and $n(z) = 2$ for all else. By substituting $h(k; z) = \psi(z+1) - 2\psi(z) + \psi(z-1) + k_{\text{lat}}^2 \psi(z)$ with $k_{\text{lat}}^2 = 2(1 - \cos(k))$, Eq. (A1) can be simplified into

$$\begin{aligned} 2k_{\text{lat}}^2 H_c^{\text{lat}}(k; L_s/2) &= (-\psi(L_s/2 + 1) + \psi(L_s/2)) \cos(kL_s/2) \\ &\quad - \psi(L_s/2) (2 \sin(kL_s/2) \sin(k)) + 2(\psi(1) - \psi(-1)). \end{aligned} \quad (\text{A3})$$

Thanks to the symmetric and periodic property of the wave function, it is easy to show that $\psi(-1) = \psi(1)$ and $\psi(L_s/2 - 1) = \psi(L_s/2 + 1)$. Using these properties, Eq. (A3) can be simplified as

$$2k_{\text{lat}}^2 H_c^{\text{lat}}(k; L_s/2) = -\psi(L_s/2) [2 \sin(kL_s/2) \sin(k)]. \quad (\text{A4})$$

In a similar way, we can obtain

$$2k_{\text{lat}}^2 H_s^{\text{lat}}(k; L_s/2) = \psi(L_s/2) [2 \cos(kL_s/2) \sin(k)]. \quad (\text{A5})$$

Taking the ratio of Eqs. (A4) and (A5), we have

$$\frac{H_s^{\text{lat}}(k; L_s/2)}{H_c^{\text{lat}}(k; L_s/2)} = \frac{-\cos(kL_s/2) \sin(k)}{\sin(kL_s/2) \sin(k)} = \cot(-kL_s/2). \quad (\text{A6})$$

By comparing this result with Eq. (75), one can see that Eq. (A6) gives Lüscher's formula, namely $\delta = -kL_s/2$.

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