Quantum phase transitions in matrix product states of one-dimensional spin-$\frac{1}{2}$ chains *

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Abstract: For the matrix product system of a one-dimensional spin-$\frac{1}{2}$ chain, we present a new model of quantum phase transitions and find that in the thermodynamic limit, both sides of the critical point are respectively described by phases $|\Psi_a\rangle=|1\cdots1\rangle$ representing all particles spin up and $|\Psi_b\rangle=|0\cdots0\rangle$ representing all particles spin down, while the phase transition point is an isolated intermediate-coupling point where the two phases coexist equally, which is described by the so-called N-qubit maximally entangled GHZ state $|\Psi_{pt}\rangle=\frac{\sqrt{2}}{2}(|1\cdots1\rangle+|0\cdots0\rangle)$. At the critical point, the physical quantities including the entanglement are not discontinuous and the matrix product system has long-range correlation and N-qubit maximal entanglement. We believe that our work is helpful for having a comprehensive understanding of quantum phase transitions in matrix product states of one-dimensional spin chains and of potential directive significance to the preparation and control of one-dimensional spin lattice models with stable coherence and N-qubit maximal entanglement.

Key words: matrix product state, quantum phase transition, long-range correlation, entanglement entropy

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1 Introduction

The study of matrix product states now mainly focuses on two aspects, one is the ability of matrix product states to characterize quantum many body systems, the other is the quantum phase transitions in matrix product systems. Related articles [1, 2] showed that for one-dimensional spin lattice models, every many-body state, in particular, every ground state (GS) of a finite many-body system dictated and characterized by a local Hamiltonian can be represented as a matrix product state (MPS). The power of this representation stems from the fact that in many cases, a low-dimensional MPS already yields a very good approximation of the state [3, 4]. Thus MPSs are undoubtedly a new powerful and convenient playground for studying one-dimensional spin lattice models theory, especially for quantum phase transitions, by using the quantum information approach [1, 5–13].

For one-dimensional spin-1 chains, our previous research [11, 12] realized the quantum phase transitions between subsystems in the composite matrix product systems, while our article [13] realized the quantum phase transition between the different special basic freedoms in the matrix product system. While in this paper, for one-dimensional spin-$\frac{1}{2}$ chains, we realize the quantum phase transition between the different special basic freedoms in the matrix product system. To be specific about the model that we construct, in the thermodynamic limit both sides of the critical point are respectively described by phases $|\Psi_a\rangle=|1\cdots1\rangle$ representing all particles spin up and $|\Psi_b\rangle=|0\cdots0\rangle$ representing all particles spin down, while the phase transition point is an isolated intermediate-coupling point where the two phases coexist equally, which is described by the so-called N-qubit maximally entangled GHZ state $|\Psi_{pt}\rangle=\frac{\sqrt{2}}{2}(|1\cdots1\rangle+|0\cdots0\rangle)$. At the critical point, the physical quantities including the entanglement are not discontinuous and the MPS $|\Psi\rangle$ has long-range correlation and N-qubit maximal entanglement due to its coherent and collective properties.

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2 Model and method

2.1 The concrete model

Let us begin with the one-dimensional translation invariant MPS:

$$|\Psi\rangle=\frac{1}{\sqrt{\mathcal{N}}}\sum_{i_1,\cdots,i_N=1}^{d}\mathrm{Tr}(A^{i_1}\cdots A^{i_N})|i_1,\cdots,i_N\rangle, \quad (1)$$

where d is the dimension of Hilbert space of one site in the spin chain, and a set of $D\times D$ matrices $\{A^i,i=1,\cdots,d\}$ parameterize the correlations of the N-spin state with the dimension $D\leqslant d^{N/2}$ [2]. $E=\sum_{i=1}^{d}\bar{A}^i\otimes A^i$ contained in the normalization factor $\mathcal{N}=\mathrm{Tr}E^N$, is the so-called transfer matrix and the symbol bar denotes complex conjugation.

Here we present the MPS $|\Psi\rangle$ with

$$A^1=\begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix},\quad A^2=\begin{bmatrix}0 & 0\\ 0 & \gamma\end{bmatrix}, \quad (2)$$

where $\gamma>0$. It is shown that the transfer matrix E has eigenvalues $1,\gamma^2,0,0$ and then $E=|\lambda_{\mathrm{a}}^{\mathrm{R}}\rangle\langle\lambda_{\mathrm{a}}^{\mathrm{L}}|+\gamma^2|\lambda_{\mathrm{b}}^{\mathrm{R}}\rangle\langle\lambda_{\mathrm{b}}^{\mathrm{L}}|$ where the normalized right (left) eigenvector $|\lambda_{\mathrm{a}}^{\mathrm{R(L)}}\rangle$ corresponds to the nonzero eigenvalue $\lambda_{\mathrm{a}}\equiv1$, and the normalized right (left) eigenvector $|\lambda_{\mathrm{b}}^{\mathrm{R(L)}}\rangle$ corresponds to the nonzero eigenvalue $\lambda_{\mathrm{b}}\equiv\gamma^2$. Obviously for $0<\gamma<1$ and $\gamma>1$, the largest absolute eigenvalue is respectively $\lambda_{\max}=\lambda_{\mathrm{a}}$ and $\lambda_{\max}=\lambda_{\mathrm{b}}$. Hence, the point $\gamma=1$ is a phase transition point. In the following, we will investigate in detail the properties of the kind of MPS QPT by the aforementioned quantum information approach.

2.2 The properties of the kind of MPS QPT

2.2.1 The properties of local physical observables

First we turn to the properties of local physical observables. For a local observable of l adjacent spins, $\boldsymbol{O}^{(1,l)}\equiv O_{i_1}^{[1]}\cdots O_{i_l}^{[l]}$ the expectation is expressed as

$$\langle\Psi|\boldsymbol{O}^{(1,l)}|\Psi\rangle=\frac{\mathrm{Tr}(E_{\boldsymbol{O}^{(1,l)}}E^{N-l})}{\mathrm{Tr}(E^N)}, \quad (3)$$

where $E_{\boldsymbol{O}^{(1,l)}}=E_{O_{i_1}}E_{O_{i_2}}\cdots E_{O_{i_l}}$ and $E_{O_k}\equiv\sum_{i,i'}\langle i|O_k|i'\rangle\bar{A}^i\otimes A^{i'}$, taking the thermodynamic limit $N\to\infty$, which reduces to

$$\langle\boldsymbol{O}^{(1,l)}\rangle=\begin{cases}\langle\boldsymbol{O}^{(1,l)}\rangle_{\mathrm{a}}=\dfrac{\langle\lambda_{\mathrm{a}}^{\mathrm{L}}|E_{\boldsymbol{O}^{(1,l)}}|\lambda_{\mathrm{a}}^{\mathrm{R}}\rangle}{(\lambda_{\mathrm{a}})^l} & \gamma<1,\\ \langle\boldsymbol{O}^{(1,l)}\rangle_{\mathrm{b}}=\dfrac{\langle\lambda_{\mathrm{b}}^{\mathrm{L}}|E_{\boldsymbol{O}^{(1,l)}}|\lambda_{\mathrm{b}}^{\mathrm{R}}\rangle}{(\lambda_{\mathrm{b}})^l} & \gamma>1,\\ \langle\boldsymbol{O}^{(1,l)}\rangle_{\mathrm{pt}}=\dfrac{1}{2}(\langle\boldsymbol{O}^{(1,l)}\rangle_{\mathrm{a}}+\langle\boldsymbol{O}^{(1,l)}\rangle_{\mathrm{b}}) & \gamma=1.\end{cases} \quad (4)$$

For simplicity, let us study the properties of the operator σ_z. The behaviors of the physical quantity $\langle\sigma_z\rangle$ for the different system size N as a function of the dimensionless parameter γ are shown in Fig. 1 and Fig. 2, where Fig. 1 is for finite N and Fig. 2 is for $N\to\infty$. Concretely, Fig. 1 shows the curves of $\langle\sigma_z\rangle$ for different N from bottom to top which takes values of 5,10,15 and 20 in turn in the vicinity of the point $\gamma=0.9$. Fig. 2 shows the behavior of $\langle\sigma_z\rangle$ for $N\to\infty$, here $\langle\sigma_z\rangle$ takes a discrete form for $0<\gamma<1$ and $\gamma>1$, it respectively takes the definite values of $\frac{1}{2}$ and $-\frac{1}{2}$ independent of the parameter γ, and when $\gamma=1$, $\langle\sigma_z\rangle=0$. It is readily seen that for the average magnetization $\langle\sigma_z\rangle$ as γ approaches 1, the degree of dependence on the parameter γ becomes stronger, while it becomes weaker with N increasing. Only in the

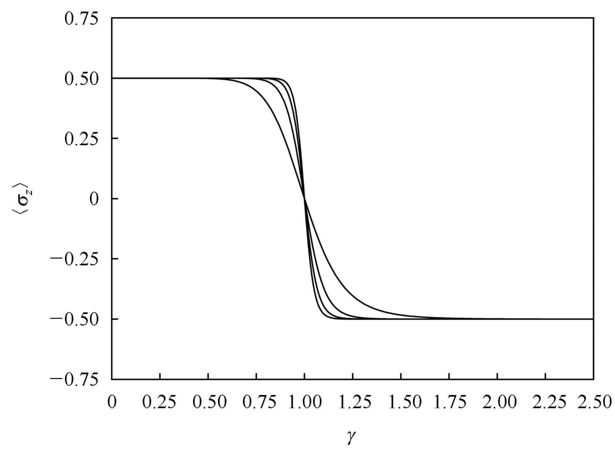

Fig. 1. The average magnetization $\langle\sigma_z\rangle$ for different values N as a function of the dimensionless parameter γ, where in the vicinity of the point $\gamma=0.9$, from bottom to top, the system size N respectively takes the values of 5, 10, 15 and 20 in turn.

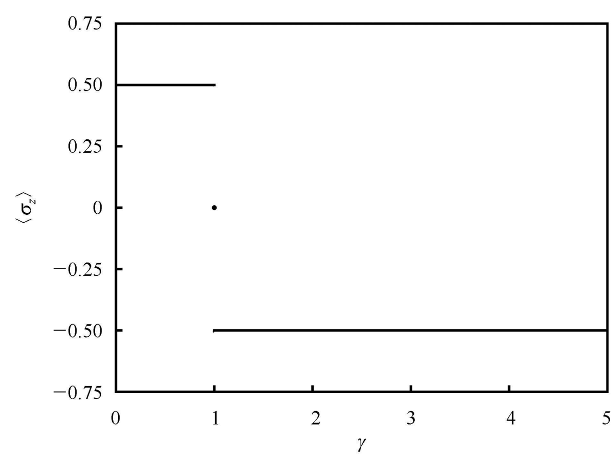

Fig. 2. The average magnetization $\langle\sigma_z\rangle$ for $N\to\infty$ as a function of the dimensionless parameter γ. When $0<\gamma<1$ and $\gamma>1$, $\langle\sigma_z\rangle$ respectively takes the value of $\frac{1}{2}$ and $-\frac{1}{2}$. When $\gamma=1$, $\langle\sigma_z\rangle=0$.

thermodynamic limit, the average magnetization $\langle\sigma_z\rangle$ turns out to be discontinuous, at the point $\gamma=1$ from Fig. 1 and Fig. 2. It follows that the phase transition can take place only in the thermodynamic limit and is clearly manifested by the singularity of the above physical quantity.

2.2.2 The property of the correlation

The property of the correlation at the transition point is discussed below. Firstly, the correlation function of two local blocks is

$$C_n[O^{(1,l)}]\equiv\langle\Psi|O^{(1,l)}O^{(n+1,n+l)}|\Psi\rangle-\langle\Psi|O^{(1,l)}|\Psi\rangle^2. \quad (5)$$

In the thermodynamic limit, for large distances $n\gg1$ and in the vicinity of the transition point, this formula reduces to

$$C_n[O^{(1,l)}] = \left(\frac{\lambda_{\mathrm{b(a)}}}{\lambda_{\mathrm{a(b)}}}\right)^n \frac{\langle\lambda_{\mathrm{a(b)}}{}^{\mathrm{L}}|E_{\boldsymbol{O}^{(1,l)}}|\lambda^{\mathrm{R}}_{\mathrm{b(a)}}\rangle\langle\lambda^{\mathrm{L}}_{\mathrm{b(a)}}|E_{\boldsymbol{O}^{(n+1,n+l)}}|\lambda^{\mathrm{R}}_{\mathrm{a(b)}}\rangle}{\lambda^{2l}_{\mathrm{a(b)}}}. \quad (6)$$

It is readily seen that from the above equation, as the coupling strength approaches its QPT, i.e., $\gamma\rightarrow1$ from either side of the critical point, we get $\lambda_{\mathrm{b}}\rightarrow\lambda_{\mathrm{a}}$, thus, the correlation length $\xi=\dfrac{1}{\ln(\lambda_{\mathrm{a(b)}}/\lambda_{\mathrm{b(a)}})}$ clearly diverges at the phase transition point. At this point, the long-range correlation is expressed as

$$C_\infty[\boldsymbol{O}^{(1,l)}]=\frac{1}{4}(\langle\boldsymbol{O}^{(1,l)}\rangle^{\mathrm{pt}}_{\mathrm{a}}-\langle\boldsymbol{O}^{(1,l)}\rangle^{\mathrm{pt}}_{\mathrm{b}})^2. \quad (7)$$

For the physical observable σ_z, the long-range correlation is $C_\infty[\sigma_z]=\frac{1}{4}$. It follows that the proposed MPS $|\Psi\rangle$ has long-range correlation at the phase transition point.

2.2.3 The entanglement property

Now, let us study the entanglement property of the MPS, the key quantity of quantum information theory [14–17], in detail. There are many kinds of methods to measure entanglement, such as the quantification characteristic function of quantum nonlocality [18], Bell inequality [19, 20], quantum discord [21], averaged entropy [22] and so on. For our system, we shall adopt the von Neumann entropy which [23–30] according to the bipartition parameterization by the adjacent spin number n of a $\mathcal{B}_n$ spin block is,

$$S_n=-\mathrm{Tr}(\rho_n\log_2\rho_n), \quad (8)$$

where $\rho_n=\mathrm{Tr}_{\bar{\mathcal{B}}_n}\rho$ is the reduced density matrix for the $\mathcal{B}_n$ block of n adjacent spins. Given an MPS, the reduced density matrix of n adjacent spins is given by

$$\rho_{i_1\cdots i_n,j_1\cdots j_n}=\frac{\mathrm{Tr}((\bar{A}_{i_1}\cdots\bar{A}_{i_n}\otimes A_{j_1}\cdots A_{j_n})E^{N-n})}{\mathrm{Tr}(E^N)}, \quad (9)$$

in the thermodynamic limit $N\rightarrow\infty$, which reduces to

$$\rho_{i_1\cdots i_n,j_1\cdots j_n}=\begin{cases}\rho^{\mathrm{a}}_{i_1\cdots i_n,j_1\cdots j_n}=\dfrac{\langle\lambda^{\mathrm{L}}_{\mathrm{a}}|\bar{A}_{i_1}\cdots\bar{A}_{i_n}\otimes A_{j_1}\cdots A_{j_n}|\lambda^{\mathrm{R}}_{\mathrm{a}}\rangle}{\lambda^n_{\max}} & \gamma<1,\\ \rho^{\mathrm{b}}_{i_1\cdots i_n,j_1\cdots j_n}=\dfrac{\langle\lambda^{\mathrm{L}}_{\mathrm{b}}|\bar{A}_{i_1}\cdots\bar{A}_{i_n}\otimes A_{j_1}\cdots A_{j_n}|\lambda^{\mathrm{R}}_{\mathrm{b}}\rangle}{\lambda^n_{\max}} & \gamma>1,\\ \rho^{\mathrm{pt}}_{i_1\cdots i_n,j_1\cdots j_k}=\dfrac{1}{2}(\rho^{a}_{i_1\cdots i_n,j_1\cdots j_n}+\rho^{\mathrm{b}}_{i_1\cdots i_n,j_1\cdots j_n}) & \gamma=1.\end{cases} \quad (10)$$

For the MPS defined by Eq. (2), considering the thermodynamic limit $N\rightarrow\infty$ concretely, the n-spin reduced density matrix reads

$$\rho_n = \begin{cases}|1\cdots1\rangle\langle1\cdots1| & \gamma<1,\\ |0\cdots0\rangle\langle0\cdots0| & \gamma>1,\\ \dfrac{1}{2}(|1\cdots1\rangle\langle1\cdots1|+|0\cdots0\rangle\langle0\cdots0|) & \gamma=1.\end{cases} \quad (11)$$

That is to say, in the thermodynamic limit $N\rightarrow\infty$, for $0<\gamma<1$ and $\gamma>1$ the n-spin state is respectively described by the pure state $|\Psi_n\rangle=|1\cdots1\rangle$ and $|\Psi_n\rangle=|0\cdots0\rangle$. When $\gamma=1$, the n-spin state is mixed state $\rho_n=\frac{1}{2}(|1\cdots1\rangle\langle1\cdots1|+|0\cdots0\rangle\langle0\cdots0|)$. According to our calculations, it is worth pointing out that whether the n spins are consecutive or not, the n-spin state is exactly the same. Then we can conclude that in the thermodynamic limit, the proposed MPS is described by

$$|\Psi\rangle=\begin{cases}|\Psi\rangle_{\mathrm{a}}=|1\cdots1\rangle & 0<\gamma<1,\\ |\Psi\rangle_{\mathrm{b}}=|0\cdots0\rangle & \gamma>1,\\ |\Psi\rangle_{\mathrm{pt}}=\dfrac{\sqrt{2}}{2}(|1\cdots1\rangle+|0\cdots0\rangle) & \gamma=1.\end{cases} \quad (12)$$

That is to say, for $0<\gamma<1$ and $\gamma>1$, the MPS $|\Psi\rangle$ is respectively in the region of phase $|\Psi_{\mathrm{a}}\rangle=|1\cdots1\rangle$ representing all particles spin up and $|\Psi_{\mathrm{b}}\rangle=|0\cdots0\rangle$ representing all particles spin down, while at the critical point, the two phases coexist equally where $|\Psi_{\mathrm{pt}}\rangle=\frac{\sqrt{2}}{2}(|1\cdots1\rangle+|0\cdots0\rangle)$ is the so-called N-qubit maximally entangled GHZ state. Hence the critical point is an isolated intermediate-coupling point consistent with the result of Fig. 2. The n-spin entanglement entropy S_n as a function of the parameter γ is as illustrated in Fig. 3. When $0<\gamma<1$ or

$\gamma>1$, S_n takes the value of 0 independent of the parameters γ and the spin number n. When $\gamma=1$, S_n takes the value of 1. It follows that at the critical point, the MPS $|\Psi\rangle$ has larger entanglement entropy and it accounts for the aforementioned long-range correlation.

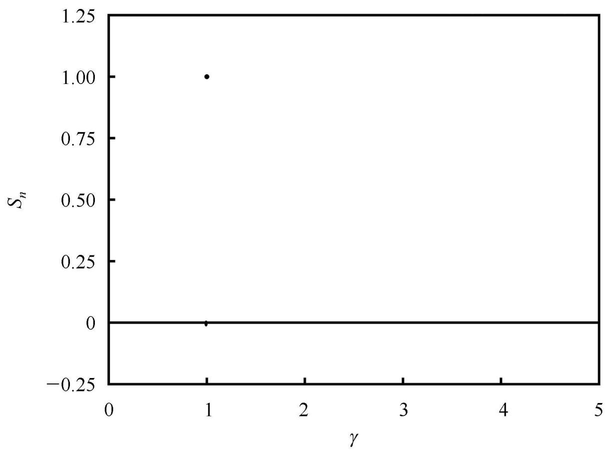

Fig. 3. The entanglement entropy of n-spin under the thermodynamic limit, S_n as a function of the dimensionless parameter γ. The entanglement entropy S_n takes the value of 1 only at the phase transition point $\gamma=1$, if not, $S_n=0$.

2.2.4 The dynamics of the specified system

Here we undertake the study of the Hamiltonian of the specified system. In general, the condition of the k-spin reduced density matrix having null space is that $d^k>D^2$. Here it only needs $k\geqslant 2$. The MPS $|\Psi\rangle$ is the GS of any Hamiltonian which is a sum of local positive operators supported in that null-space. Thinking along this line, we can always construct a local Hamiltonian such that a given MPS is its GS. Without the loss of generality, such a Hamiltonian is mathematically expressed as

$$H=\sum_i u_i(P_k), \tag{13}$$

with P_k being the projector onto the null-space of ρ_k and $u_i>0$ its translation to site i. In terms of the proposed system in the thermodynamic limit, the Hamiltonian is described by

$$H=\begin{cases} H_{\rm a}=\sum\limits_{i=1}^{N}2-\sigma_i^z-\sigma_{i+1}^z & 0<\gamma<1,\\ H_{\rm pt}=\sum\limits_{i=1}^{N}I-\sigma_i^z\sigma_{i+1}^z & \gamma=1,\\ H_{\rm b}=\sum\limits_{i=1}^{N}2+\sigma_i^z+\sigma_{i+1}^z & \gamma>1.\end{cases} \tag{14}$$

By construction, the GS energy is always zero, i.e., it is evidently analytic in γ and moreover $|\Psi\rangle$ is its unique GS for either side of the critical point discussed in Refs. [1, 8, 31]. The analyticity of the Hamiltonian ground state energy and the uniqueness of its GS for either side of the critical point immediately imply that a nonanalyticity in the physical quantities can only be caused by a vanishing energy gap at the transition points.

2.2.5 The long-wavelength behavior

In order to have a comprehensive and deeper understanding of the kind of MPS QPT, we study below the scaling property. Specifically, we resort to a renormalization group approach to characterize the long-wavelength behavior of the specified system. Similar to the standard Kadanof Blocking scheme, the coarse-graining procedure for matrix product states could be achieved by merging the representative matrices of neighboring sites as $A\rightarrow A^{(\rm pq)}\equiv A^{\rm p}A^{\rm q}$ and subsequently performing a fine-grained transformation $A\rightarrow A'$ to select out new representatives [32]. The transfer matrix in every step transforms as $E\rightarrow E'\equiv E^2$ and an iterative process hence leads to a fixed point $E^{\infty}\equiv E^{\rm fp}$ in which only the vector(s) of largest eigenvalue(s) can survive. In terms of the MPS $|\Psi\rangle$ under consideration, the normalized transfer operator of the fixed point is, respectively, $E^{\rm fp}=|\lambda_{\rm a}^{\rm R}\rangle\langle\lambda_{\rm a}^{\rm L}|$ and $E^{\rm fp}=|\lambda_{\rm b}^{\rm R}\rangle\langle\lambda_{\rm b}^{\rm L}|$ for $0<\gamma<1$ and $\gamma>1$, and the corresponding representative matrices of the fixed point are obtained as $\{A_{\rm fp}^i\}=\{A_{\rm a(fp)}^i, i=1,2\}$ and $\{A_{\rm fp}^i\}=\{A_{\rm b(fp)}^i, i=1,2\}$ where

$$\{A_{\rm a(fp)}^i\}=\left\{\begin{bmatrix}1&0\\0&0\end{bmatrix},\begin{bmatrix}0&0\\0&0\end{bmatrix}\right\} \tag{15}$$

which represent all particles spin up and

$$\{A_{\rm b(fp)}^i\}=\left\{\begin{bmatrix}0&0\\0&0\end{bmatrix},\begin{bmatrix}0&0\\0&1\end{bmatrix}\right\} \tag{16}$$

all particles spin down. When $\gamma=1$, the corresponding fixed point of the MPS $|\Psi\rangle$ is characterized by the normalized $E_{\rm pt}^{\rm fp}=|\lambda_{\rm a}^{\rm R}\rangle\langle\lambda_{\rm a}^{\rm L}|+|\lambda_{\rm b}^{\rm R}\rangle\langle\lambda_{\rm b}^{\rm L}|$ and the corresponding representative matrices of the fixed point are

$$\{A_{\rm pt(fp)}^i\}=\left\{\begin{bmatrix}1&0\\0&0\end{bmatrix},\begin{bmatrix}0&0\\0&1\end{bmatrix}\right\} \tag{17}$$

which represent the two phases coexisting equally described by the so-called N-qubit maximally entangled GHZ state and stands distinctly for an isolated intermediate-coupling phase transition point. That is to say, the fixed point state $|\Psi_{\rm fix}\rangle$ of the specified system is described by

$$|\Psi_{\rm fp}\rangle=\begin{cases}|\Psi_{\rm a(fp)}\rangle=|1\cdots1\rangle & 0<\gamma<1,\\ |\Psi_{\rm b(fp)}\rangle=|0\cdots0\rangle & \gamma>1,\\ |\Psi_{\rm pt(fp)}\rangle=\dfrac{\sqrt{2}}{2}(|1\cdots1\rangle+|0\cdots0\rangle) & \gamma=1.\end{cases} \tag{18}$$

The results reconfirm the above conclusions about the kind of phase transition.

3 Conclusions

In conclusion, MPSs provide an effective tool for investigating novel types of quantum phase transitions. Here we present a new kind of quantum phase transition in matrix product states of one-dimensional spin-$\frac{1}{2}$ chains and find that in the thermodynamic limit, both sides of the critical point are respectively described by phases $|\Psi_{\rm a}\rangle=|1\cdots1\rangle$ representing all particles spin up and $|\Psi_{\rm b}\rangle=|0\cdots0\rangle$ representing all particles spin down, while the phase transition point is an isolated intermediate-coupling point where the two phases coexist equally, which is described by the so-called N-qubit maximally entangled GHZ state

$$|\Psi_{\rm pt}\rangle=\frac{\sqrt{2}}{2}(|1\cdots1\rangle+|0\cdots0\rangle).$$

At the critical point, the physical quantities including the entanglement are not discontinuous and the MPS has long-range correlation and N-qubit maximal entanglement due to its coherent and collective properties. We believe that our work is helpful for having a comprehensive understanding of the quantum phase transitions in matrix product states of one-dimensional spin chains and of potential directive significance to the preparation and control of one-dimensional spin lattice models with stable coherence and N-qubit maximal entanglement.

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