Quantum phase transitions about parity breaking in matrix product systems*

ZHU Jing-Min(祝敬敏)1)

College of Optoelectronic Technology, Chengdu University of Information Technology, Chengdu 610225, China

Abstract: According to our scheme to construct quantum phase transitions (QPTs) in spin chain systems with matrix product ground states, we first successfully combine matrix product state (MPS) QPTs with spontaneous symmetry breaking. For a concrete model, we take into account a kind of MPS QPTs accompanied by spontaneous parity breaking, though for either side of the critical point the GS is typically unique, and show that the kind of MPS QPTs occur only in the thermodynamic limit and are accompanied by the appearance of singularities, diverging correlation length, vanishing energy gap and the entanglement entropy of a half-infinite chain not only staying finite but also whose first derivative discontinuous.

Key words: matrix product state, quantum phase transitions, parity breaking, entanglement entropy

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1 Introduction

The study of quantum many-body systems is a much more intensive research subject in the field of condensed matter due to the richness of inherent complexity of a large number of interacting particles, among which quantum phase transitions (QPTs) occupy a distinguished position. These transitions, taking place at zero temperature, are driven by fluctuations due to the Heisenberg uncertainty principle even in the ground states (GSs) [1].

However, related articles [2, 3] showed that every state, in particular, every GS, of a finite system characterized by 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 [4]. MPSs are therefore undoubtedly a convenient playground for studying quantum many-body systems, especially for investigating QPTs by the quantum information approach [2, 5, 6] which deals with primarily quantum states, from which corresponding parent Hamiltonians may be constructed such that the quantum states arise as exact GSs. M Fannes et al. and others [2, 7] already indicated the possibility of such transitions in MPS systems, in quasi-exactly solvable models. Michael M. Wolf et al. [8] generalized the finding of the MPS QPTs and showed how to engineer the QPT points between phases with predetermined properties, and pointed out that these MPS QPTs take place only in the thermodynamic limit and are accompanied by the appearance of singularities, diverging correlation length, vanishing energy gap and other features which differ from the standard paradigm: (i) the ground state energy remains analytic, (ii) the entanglement entropy of a half-infinite chain stays finite, and (iii) MPS QPTs can occur without spontaneous symmetry breaking since for either side of the critical point the GS is typically unique.

According to our scheme to construct various quantum phase transitions (QPTs) in spin chain systems with matrix product ground states [9], we first successfully combine the matrix product state (MPS) QPTs with spontaneous symmetry breaking. For a concrete model, we take into account the kind of MPS QPTs accompanied by spontaneous parity breaking, though for either side of the critical point the GS is typically unique. We also study the properties of the concrete model, and show that, the kind of MPS QPTs take place only in the thermodynamic limit and are accompanied by the appearance of singularities,

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1) E-mail: zhujm66@yahoo.com

diverging correlation length, vanishing energy gap and the entanglement entropy of a half-infinite chain not only staying finite but also whose first derivative is discontinuous and other aforementioned features which differ from the standard paradigm [2, 7, 8].

2 Model and method

The 1D translation invariant MPS is given by

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

where d is the Hilbert space dimension of one-spin in the chain and the set of $D\times D$ matrices $\{A^i, i=1,\cdots,d\}$ parameterize the N-spin state with the dimension $D\leqslant d^{N/2}$. The normalization factor is obtained as $\mathcal{N}=\mathrm{Tr}(E^N)$, where $E=\sum_{i=1}^{d}\bar{A}^i\otimes A^i$ is the so-called transfer matrix with the bar denoting complex conjugation. Supposing that the MPSs $|\Psi_\mathrm{a}\rangle$ and $|\Psi_\mathrm{b}\rangle$ are represented respectively by the set of matrices $\{A_\mathrm{a}^i\}=\{A_\mathrm{a}^1,A_\mathrm{a}^2\cdots A_\mathrm{a}^d\}$ and $\{A_\mathrm{b}^i\}=\{A_\mathrm{b}^1,A_\mathrm{b}^2\cdots A_\mathrm{b}^d\}$, we can construct a new MPS

$$\begin{aligned}|\Psi\rangle &= \frac{1}{\sqrt{\mathcal{N}}}\sum_{x=\mathrm{a,b}}\sum_{i_1,\cdots,i_N=1}^{d}\mathrm{Tr}(A_x^{i_1}\cdots A_x^{i_N})|i_1,\cdots,i_N\rangle\\ &= \frac{1}{\sqrt{\mathcal{N}}}\sum_{i_1,\cdots,i_N=1}^{d}\mathrm{Tr}(A^{i_1}\cdots A^{i_N})|i_1,\cdots,i_N\rangle, \quad (2)\end{aligned}$$

where obviously $A^i=A_\mathrm{a}^i\oplus A_\mathrm{b}^i$. The transfer matrix E contained in $\mathcal{N}$ possesses definitely the similarity relation $E\sim E_\mathrm{a}\oplus E_\mathrm{ab}\oplus E_\mathrm{ba}\oplus E_\mathrm{b}$, where $E_{\mathrm{a(b)}}$ are the corresponding transfer matrices of $|\Psi_{\mathrm{a(b)}}\rangle$ and $E_\mathrm{ab}\equiv\sum_i\bar{A}_\mathrm{a}^i\otimes A_\mathrm{b}^i$. As will be specified in detail later, the established special linear combination of relational MPSs regime for quantum many-body states undoubtedly is a convenient and effective scheme to construct and investigate various quantum phase transitions. In this paper, by using the scheme, we will take into account a kind of MPS QPTs appearance accompanied by spontaneous symmetry breaking.

2.1 The properties of the kind of MPS QPT

Now let us introduce in detail the kind of MPS QPT appearance with spontaneous symmetry breaking and study the kind of phase transition phenomena by the aforementioned quantum information approach. For a concrete example, first let us consider a parity conserved MPS $|\Psi_\mathrm{a}\rangle$ with

$$A_\mathrm{a}^1=\begin{bmatrix}1&0\\0&1\end{bmatrix},\ A_\mathrm{a}^2=\begin{bmatrix}0&1\\0&0\end{bmatrix},\ A_\mathrm{a}^3=\begin{bmatrix}0&0\\1&0\end{bmatrix}, \quad (3)$$

and a MPS $|\Psi_\mathrm{b}\rangle$ with

$$A_\mathrm{b}^1=\begin{bmatrix}1&0\\0&\gamma\end{bmatrix},\ A_\mathrm{b}^2=\begin{bmatrix}0&1\\0&0\end{bmatrix},\ A_\mathrm{b}^3=\begin{bmatrix}0&0\\\gamma&0\end{bmatrix}, \quad (4)$$

where $\gamma\geqslant 0$. When the dimensionless parameter γ is not $0,1$, we know that the MPS $|\Psi\rangle_\mathrm{b}$ is parity nonconserving [10, 11]. Then we construct the MPS $|\Psi\rangle$, where its representative matrices are $A^i=A_\mathrm{a}^i\oplus A_\mathrm{b}^i (i=1,\ 2,\ 3)$. We now study in detail the properties of the MPS $|\Psi\rangle$ constructed above. The two largest absolute eigenvalues of the transfer matrix E for this case are $\lambda_\mathrm{a}=2$ with the normalized right and left eigenvectors $|\lambda_\mathrm{a}^\mathrm{R}\rangle$ and $|\lambda_\mathrm{a}^\mathrm{L}\rangle$ and $\lambda_\mathrm{b}=1+\gamma^2$ with the normalized right and left eigenvectors $|\lambda_\mathrm{b}^\mathrm{R}\rangle$ and $|\lambda_\mathrm{b}^\mathrm{L}\rangle$, respectively corresponding to E_a and E_b. Here for $0\leqslant\gamma<1$ and $\gamma>1$, the largest absolute eigenvalue is respectively λ_a and λ_b; that is to say, in the thermodynamic limit, $|\Psi\rangle$ is respectively in the region of the phase $|\Psi_\mathrm{a}\rangle$ and $|\Psi_\mathrm{b}\rangle$ correspondingly. Hence, the point $\gamma=1$ is a point of phase transition. The expectation of the parity operator P_N under the thermodynamic limit, $\langle P_N\rangle$ is 1 in one phase and 0 in the other for $0\leqslant\gamma\leqslant 1$ and $\gamma>1$, respectively, as shown in Fig. 1; therefore, it is an order parameter which signals a quantum phase transition accompanied by spontaneous parity breaking at the point $\gamma=1$.

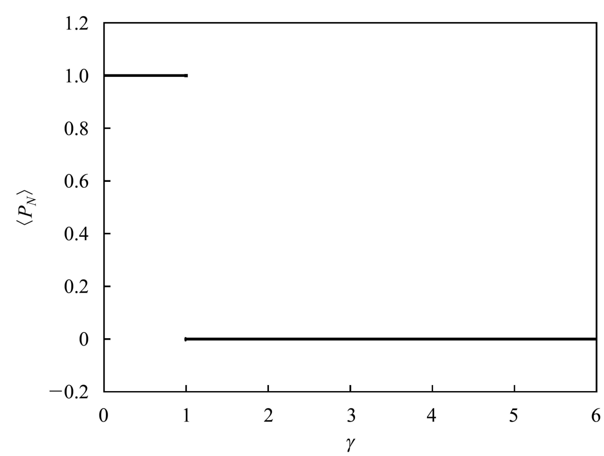

Fig. 1. The expectation value of the parity operator under the thermodynamic limit, $\langle P_N\rangle$ as a function of the dimensionless parameter γ. $\langle P_N\rangle$ is 1 in one phase and 0 in the other for $0\leqslant\gamma\leqslant 1$ and $\gamma>1$, respectively.

Now 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

$$\langle\Psi|\boldsymbol{O}^{(1,l)}|\Psi\rangle=\frac{\mathrm{Tr}(E_{\boldsymbol{O}^{(1,l)}}E^{N-l})}{\mathrm{Tr}(E^N)}, \quad (5)$$

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

$$\langle \boldsymbol{O}^{(1,l)}\rangle = \begin{cases} \langle \boldsymbol{O}^{(1,l)}\rangle_{\rm a} = \dfrac{\langle \lambda_{\rm a}^{\rm L}|E_{\boldsymbol{O}^{(1,l)}}|\lambda_{\rm a}^{\rm R}\rangle}{(\lambda_{\rm a})^l},\ \gamma\leqslant 1, \\ \langle \boldsymbol{O}^{(1,l)}\rangle_{\rm b} = \dfrac{\langle \lambda_{\rm b}^{\rm L}|E_{\boldsymbol{O}^{(1,l)}}|\lambda_{\rm b}^{\rm R}\rangle}{(\lambda_{\rm b})^l},\ \gamma > 1. \end{cases} \tag{6}$$

For simplicity, let us study the properties of the operator J_z at the critical point. The behaviors of the physical quantity $\langle J_z\rangle$ for different values N as a function of the dimensionless parameter γ, are shown in Fig. 2, where, in the vicinity of the point $\gamma=0.75$, from top to bottom the curves represent the curve of $\langle J_z\rangle$ with N taking values of $5, 10, 15, 20$ and ∞ in turn. It is readily seen that only in the thermodynamic limit, the first derivative of the average magnetization $\langle J_z\rangle$ turns out to be discontinuous, at the point $\gamma=1$ from Fig. 2. It follows that the phase transition between phases $|\Psi_{\rm a}\rangle$ and $|\Psi_{\rm b}\rangle$ can take place only in the thermodynamic limit and is clearly manifested by singularity of the above physical quantity.

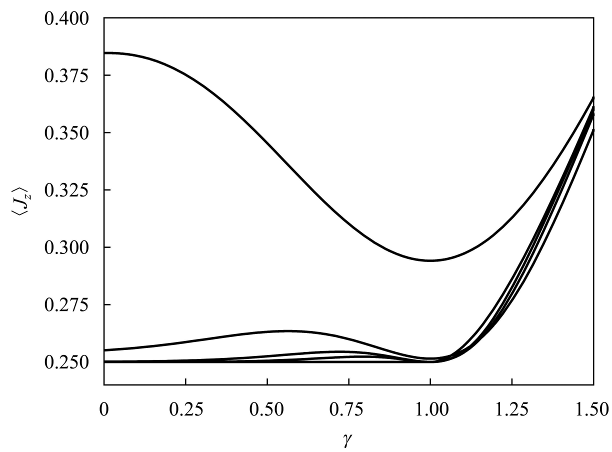

Fig. 2. The average magnetization $\langle J_z\rangle$ for different values N as a function of the dimensionless parameter γ. In the vicinity of the point $\gamma=0.75$, from top to bottom the curves represent the curve of $\langle J_z\rangle$ with N taking values of 5, 10, 15, 20 and ∞ in turn. Only in the thermodynamic limit, the first derivative of the average magnetization $\langle J_z\rangle$ turns out to be discontinuous, at the point $\gamma=1$.

The properties of the correlation in the vicinity of the transition point are discussed below. Firstly, the correlation function of two local blocks is

$$C_n[O^{(1,l)}]\equiv\langle\Psi|O^{(1,l)}O^{(n+1,n+l)}|\Psi\rangle-\langle\Psi|O^{(1,l)}|\Psi\rangle^2. \tag{7}$$

In the thermodynamic limit, for large distances $n\gg 1$ and in the vicinity of the transition point, this formula reduces to

$$C_n[O^{(1,l)}]=\left(\frac{\lambda_{\rm b(a)}}{\lambda_{\rm a(b)}}\right)^n \times\frac{\langle\lambda_{\rm a(b)}{}^{\rm L}|E_{\boldsymbol{O}^{(1,l)}}|\lambda^{\rm R}_{\rm b(a)}\rangle\langle\lambda^{\rm L}_{\rm b(a)}|E_{\boldsymbol{O}^{(n+1,n+l)}}|\lambda^{\rm R}_{\rm a(b)}\rangle}{\lambda^{2l}_{\rm a(b)}}. \tag{8}$$

It is readily seen that from the above equation, as the coupling strength approaches its QPT, i.e., $\gamma\to1$ from either side of the critical point, we get $\lambda_{\rm b}\to\lambda_{\rm a}$, thus, the correlation length $\xi=\dfrac{1}{\ln(\lambda_{\rm a(b)}/\lambda_{\rm b(a)})}$ clearly diverges at the phase transition point.

Here we undertake the study of the Hamiltonian of the specified system. Given a MPS, the reduced density matrix of k adjacent spins is given by

$$\rho_{i_1\cdots i_k,j_1\cdots j_k}=\frac{{\rm Tr}((\bar{A}_{i_1}\cdots\bar{A}_{i_k}\otimes A_{j_1}\cdots A_{j_k})E^{N-k})}{{\rm Tr}(E^N)}, \tag{9}$$

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

$$\rho_{i_1\cdots i_k,j_1\cdots j_k}=\begin{cases}\rho^{\rm a}_{i_1\cdots i_k,j_1\cdots j_k}=\dfrac{\langle\lambda^{\rm L}_{\rm a}|\bar{A}_{i_1}\cdots\bar{A}_{i_k}\otimes A_{j_1}\cdots A_{j_k}|\lambda^{\rm R}_{\rm a}\rangle}{\lambda^k_{\max}}\ \ \gamma\leqslant1,\\ \rho^{\rm b}_{i_1\cdots i_k,j_1\cdots j_k}=\dfrac{\langle\lambda^{\rm L}_{\rm b}|\bar{A}_{i_1}\cdots\bar{A}_{i_k}\otimes A_{j_1}\cdots A_{j_k}|\lambda^{\rm R}_{\rm b}\rangle}{\lambda^k_{\max}}\ \ \gamma>1.\end{cases} \tag{10}$$

This density matrix has at least d^k-D^2 zero eigenvalues (of course, it is sufficient that the following inequality holds: $d^k>D^2$). We can always construct a local Hamiltonian such that a given MPS is its GS. Therefore, $|\Psi\rangle$ is the GS of any Hamiltonian which is a sum of local positive operators supported in that null-space. In particular, it is the GS of the Hamiltonian

$$H=\sum_i u_i(P_k), \tag{11}$$

with P_k being the projector onto the null-space of ρ_k and u_i its translation to site i. Obviously, the Hamiltonian under the thermodynamic limit, takes a discrete form, namely, for $\gamma\leqslant1$ and $\gamma>1$, $H=H_{\rm a}$ and $H=H_{\rm b}$, where $H_{\rm a}=H_{\rm b}(\gamma=1)$. One form of $H_{\rm b}$ is

$$\begin{aligned}H_{\rm b}\ =\ &\sum_i\left(\frac{\gamma^2+2\gamma^4}{4}(S^i_z(S^{i+1}_z)^2)+\frac{\gamma^2+2}{4}(S^i_z)^2S^{i+1}_z\right.\\ &-\gamma^3(S^i_zS^i_+(S^{i+1}_+)^2+S^i_-S^i_z(S^{i+1}_-)^2)\\ &-\gamma((S^i_+)^2S^{i+1}_zS^{i+1}_++(S^i_-)^2S^{i+1}_-S^{i+1}_z)\\ &+\gamma^2(S^i_+S^i_zS^{i+1}_zS^{i+1}_-+S^i_zS^i_-S^{i+1}_+S^{i+1}_z)\\ &+\frac{\gamma^2-2\gamma^4-2}{4}(S^i_z)^2(S^{i+1}_z)^2+\frac{\gamma^2}{4}S^i_zS^{i+1}_z\end{aligned}$$

$$+\frac{1}{2}((S_z^{i+1})^2-S_z^{i+1})+\frac{\gamma^4}{2}((S_z^i)^2-S_z^i)), \quad (12)$$

where $S_z=|+\rangle\langle+|-|-\rangle\langle-|, S_+=\frac{\sqrt{2}}{2}(S_x+\mathrm{i}S_y)$ and $S_-=\frac{\sqrt{2}}{2}(S_x-\mathrm{i}S_y)$. The above expressions characterize that $H=H_\mathrm{a}$ has parity symmetry and $H=H_\mathrm{b}$ is parity non-conserving respectively. 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. [2, 8, 12]. The analyticity of H 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 point.

In order to have a comprehensive and deeper understanding of the kind of MPS QPT, we study below the property of the fixed point and the scaling property of entanglement, the key quantity of quantum information theory [13–16]. Specifically, we resort to 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 $A\rightarrow A^{(\mathrm{pq})}\equiv A^\mathrm{p}A^\mathrm{q}$ and subsequently performing a fine-grained transformation $A\rightarrow A'$ to select out new representatives [17]. The transfer matrix in every step transforms as $E\rightarrow E'\equiv E^2$ and an iterative process hence leads to a fixed point $E^\infty\equiv E^\mathrm{fp}$ 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, $E^\mathrm{fp}=|\lambda_\mathrm{a}^\mathrm{R}\rangle\langle\lambda_\mathrm{a}^\mathrm{L}|$ and $E^\mathrm{fp}=|\lambda_\mathrm{b}^\mathrm{R}\rangle\langle\lambda_\mathrm{b}^\mathrm{L}|$ for $0\leqslant\gamma\leqslant1$ and $\gamma>1$, and the corresponding representative matrices of the fixed point are obtained as $\{A_\mathrm{fp}^i\}=\{A_{\mathrm{a(fp)}}^i\}$, $i=1,\cdots,4\}$ and $\{A_\mathrm{fp}^i\}=\{A_{\mathrm{b(fp)}}^i$, $i=1,\cdots,4\}$ where

$$\{A_{\mathrm{a(fp)}}^i\}=\left\{\begin{bmatrix}1&0\\0&0\end{bmatrix},\begin{bmatrix}0&1\\0&0\end{bmatrix},\begin{bmatrix}0&0\\1&0\end{bmatrix},\begin{bmatrix}0&0\\0&1\end{bmatrix}\right\} \quad (13)$$

and

$$\{A_{\mathrm{b(fp)}}^i\}=\left\{\begin{bmatrix}1&0\\0&0\end{bmatrix},\begin{bmatrix}0&1\\0&0\end{bmatrix},\begin{bmatrix}0&0\\\gamma&0\end{bmatrix},\begin{bmatrix}0&0\\0&\gamma\end{bmatrix}\right\} \quad (14)$$

are respectively the representative matrices of the MPSs $|\Psi_\mathrm{a}^\mathrm{fp}\rangle$ and $|\Psi_\mathrm{b}^\mathrm{fp}\rangle$ representing the fixed point of the MPSs $|\Psi_\mathrm{a}\rangle$ and $|\Psi_\mathrm{b}\rangle$. That is to say, the fixed point state of the specified system is respectively $|\Psi^\mathrm{fp}\rangle=|\Psi_\mathrm{a}^\mathrm{fp}\rangle$ and $|\Psi^\mathrm{fp}\rangle=|\Psi_\mathrm{b}^\mathrm{fp}\rangle$ for $0\leqslant\gamma\leqslant1$ and $\gamma>1$. The depicted renormalization group fixed point enables a convenient calculation of the entanglement entropy between one half-infinite chain and the other which is equivalent to the entanglement entropy between the bipartite coarse-grained spins of the fixed point, because they belong to an equivalence class of D-dimensional MPSs where all elements of the class are related by local unitary operations. In detail, the entanglement entropy between the bipartite coarse-grained spins is, respectively,

$$S=-\mathrm{Tr}(\rho^1\log_2\rho^1)=-\mathrm{Tr}(\rho_\mathrm{a}^1\log_2\rho_\mathrm{a}^1)=2, \quad (15)$$

and

$$\begin{aligned}S&=-\mathrm{Tr}(\rho^1\log_2\rho^1)=-\mathrm{Tr}(\rho_\mathrm{b}^1\log_2\rho_\mathrm{b}^1)\\&=\frac{2+4\gamma^2+\gamma^4}{(1+\gamma^2)^2}\log_2(1+\gamma^2)-\frac{4\gamma^2+2\gamma^4}{(1+\gamma^2)^2}\log_2\gamma, \quad (16)\end{aligned}$$

for $0\leqslant\gamma\leqslant1$ and $\gamma>1$. Fig. 3 shows the behavior of the entanglement entropy between the bipartite coarse-grained spins of the fixed point, i.e., one half-infinite chain and the other, S as a function of the dimensionless parameter γ. It is obvious that at the phase transition point $\gamma=1$, the entanglement entropy between one half-infinite chain and the other, takes the value of 2, which implies that the entanglement entropy of a half-infinite chain stays finite reflecting the fact that MPS QPTs cannot be described in terms of conformal field theory [8, 18], and the first derivative of it is discontinuous.

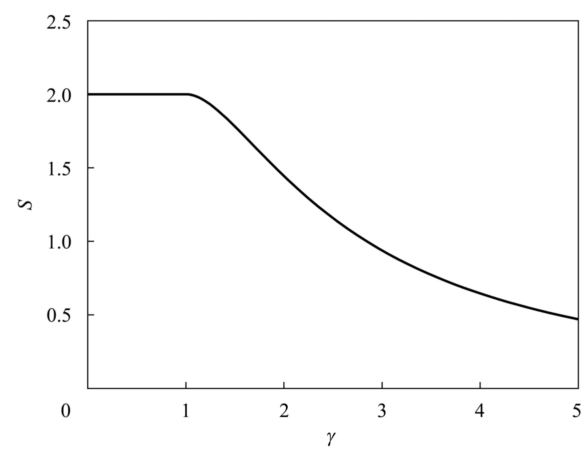

Fig. 3. The entanglement entropy between one half-infinite chain and the other, S as a function of the dimensionless parameter γ. At the phase transition point $\gamma=1$, the entanglement entropy between one half-infinite chain and the other, takes the value of 2 and the first derivative of it is discontinuous.

2.2 Brief summary

These facts show that this kind of MPS QPTs take place only in the thermodynamic limit and is accompanied by the appearance of singularities, diverging correlation length, vanishing energy gap, and other properties including that the ground state energy remains analytic, and the entanglement entropy of a half-infinite chain not only stays finite but also the first derivative of it is discontinuous. In a word, what is more important is that this kind of MPS QPTs can occur, accompanied by spontaneous symmetry breaking, though for either side of the critical point the GS is typically unique.

3 Conclusions

In conclusion, MPSs provide an effective tool for investigating novel types of quantum phase transitions that do not fit in the traditional framework. We presented a new general and simple scheme to construct various quantum phase transitions in spin chain systems with matrix product ground states using a kind of special linear combination of relational MPSs regime. It is worth pointing out that this scheme has the advantage of combining MPS QPTs with spontaneous symmetry breaking and based on the idea of this scheme, one may investigate more diverse kinds of quantum phase transitions which deserve to be investigated in future research.

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