Path selection rule in matrix product systems

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A matrix product system chooses a special path in the phase diagram to undergo a quantum phase transition (QPT) and shows different behaviors compared with a traditional QPT, such as the symmetry behavior of some physical observables described in this paper. An equation is established, which (i) helps one to understand the special behaviors of a matrix product state (MPS)-QPTs, and (ii) can be used to detect the QPT point of a MPS, much simpler than usual procedures of calculating the transfer matrix or density matrix of the system. The equation acts as a selection rule for the path of the MPS-QPT and is believed to be the essence of distinguishing a MPS-QPT from a traditional QPT. Furthermore, the discontinuity of the derivative of an observable is found to be connected directly to the turning point in the path of the MPS, but not the phase boundary point in the phase diagram, though the two are in accordance with each other in many cases.

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I. INTRODUCTION

In systems with a large number of interacting particles, many complex and interesting phenomena arise, among which quantum phase transitions (QPTs) occupy a distinguished position. For example, a magnetic system may show a QPT when an appropriate magnetic field is imposed. In the vicinity of the transition point, the derivative of the observable with respect to the external parameter is discontinuous and the correlation length is divergent, which are considered to be indicators of a traditional QPT.[1]

Recently, QPTs in quantum spin chain systems characterized by local Hamiltonians with matrix product ground states are investigated by many groups.[2–7] Suppose one has a closed spin chain with N sites and let d be the dimension of the Hilbert space ω at each site. Then unnormalized matrix product states (MPSs) are defined as

$$|\psi(g)\rangle = \sum_{i_1,\ldots,i_N=1}^{d} \mathrm{tr}(A_{i_1},\ldots,A_{i_N})|i_1,\ldots,i_N\rangle,$$

where the A_j's, with $j=1,\ldots,d$, are $D\times D$ matrices; D is the dimension of the bonds in the so-called valence bond picture.[8–10] We focus on $D=2$ in this paper. We assume that the matrices $A_j := A_j(g)$ depend on one or more parameters generically denoted by g. In addition, we only consider translationally invariant states, by taking the matrices to be site independent. For a given MPS, one can always construct a parent Hamiltonian which guarantees the MPS be its ground state.[2] One can use transfer matrix method[2,5] to calculate the density matrix of the system, then all physical observables can be calculated. With these observables, two schemes are used to detect a MPS-QPT: one is to consider the analyticity of the derivative of an observable (i.e., average magnetization, measures of quantum entanglement,[4,5,11] two-particle functions) and the other concerns with the divergence of the correlation length or the vanishing of the fidelity.[3,7,12]

It has been pointed out that a MPS-QPT differs from a traditional QPT in some aspects.[2] For example, the ground-state energy remains analytic in a MPS-QPT while shows a singular point in a traditional QPT. In addition to these differences, we find an interesting phenomenon. In a traditional phase transition, observables are generally not symmetrical with respect to the critical point $g=g_c$ [see Fig. 1(a) (bottom)]. A typical example was reported in our recent publication[13] investigating the QPTs of spin-$\frac{1}{2}$ diamond models, where neither the magnetization nor the quantum entanglement of the system shows any symmetry behavior in the vicinity of QPT points. In contrast, one can find that in many MPSs some quantities are symmetrical with respect to the MPS-QPT point g_c. For spin ladders with SO(2) symmetry (rotation around the z axis in spin space) and three Z_2 symmetries (spin flip, parity, and leg exchange),[5] the correlation function G_z is found to be symmetrical with respect to g_c and similar results can be found in the q-deformed valence bond solid (VBS) model.[14] For XYZ spin chains with matrix product ground state,[6] the average magnetization in the x direction is symmetrical with respect to g_c. In spin liquid models,[7] the single-site von Neumann entropy and the two-site entropy are symmetrical with respect to g_c.

As the symmetry behavior is observed in many matrix product systems, the intention of this paper is to investigate the intrinsic origin of this phenomenon. We find that this symmetry of a MPS, as well as the particular analyticity of the ground-state energy mentioned above, can be well understood by considering the special path along which a MPS evolves in the phase diagram.[15] We characterize the path by an equation called the symmetry equation in this paper. The equation can be used to judge whether a MPS has such a symmetry point or not and identify its location if it has. We find that the symmetry point is usually the singular point of a physical observable, thus the equation can help us to detect the MPS-QPT point. Examples show that this method is much simpler than usual procedures of calculating the transfer matrix or density matrix of the system. In addition, the MPS-QPT point is found to be connected directly to the turning point in the path of the MPS, but not necessarily the phase boundary point in the phase diagram; thus, there may be no traditional *phase transition* at all in some MPS-QPTs. Finally, we will discuss a complex case, that is, a physical observable can show a global symmetry point and several local symmetry points in some systems.

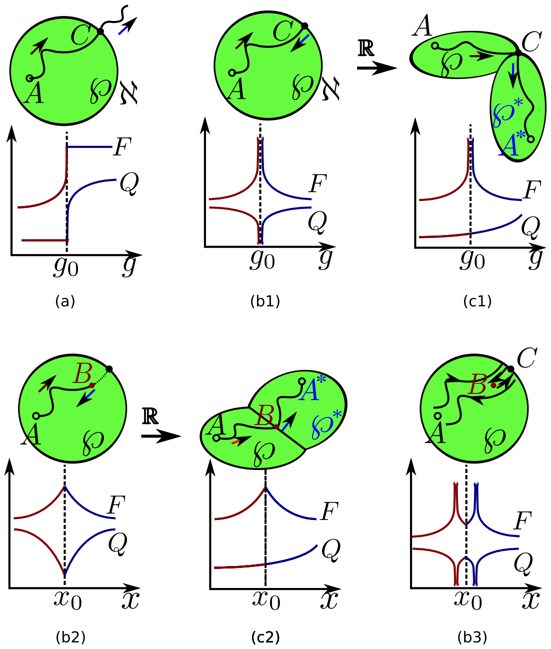

FIG. 1. (Color online) Phase diagram (top) and physical observables (bottom) for several models. Two phases are marked as $\wp$ and $\aleph$ with the boundary indicated by the circle. F and Q denote some physical observables. (a) In a traditional QPT, the system crosses the boundary through a normal path, then a singular point would be observed and usually no symmetry would be observed. (b1) For a trivial MPS with $\mathbb{R}=\mathbb{I}$, the states $|\psi(g_0-\xi)\rangle$ and $|\psi(g_0+\xi)\rangle$ at the two sides of the symmetry point g_0 correspond to the same point in the phase diagram. (c1) For $\mathbb{R}\neq\mathbb{I}$, the system strides over two phases through a special path, where its path in $\wp^*$ can be imagined as the "rotation" (corresponding to the unitary transformation $\mathbb{R}$ in the symmetry equation) of its path in $\wp$. (b2) A trivial model (with $\mathbb{R}=\mathbb{I}$) is constructed to show that a (trivial) symmetry point can deviate from phase boundary due to some mathematical reasons. By rotating (b2), we get a intuitive image that in a nontrivial MPS (with $\mathbb{R}\neq\mathbb{I}$) a singularity may be observed at any turning point in the path of the MPS, shown in (c2). (b3) We use another trivial model to illustrate that multiple symmetry points may be observed due to mathematical reasons. By rotating (b3), one can easily imagine the path of the complex q-deformed spin-1 MPS, which is a nontrivial model showing three symmetry points.

The structure of this paper is as follows: in Sec. II we propose a symmetry equation to explain the symmetry behavior of MPSs. In Sec. III we investigate in detail two representative examples with our theory and draw corresponding paths in the phase diagram. In Sec. IV the relationship between the singularity of a physical observable and the phase boundary point in the phase diagram is discussed. We study multiple-symmetry-point MPSs in Sec. V and a conclusion is given in Sec. VI.

II. SYMMETRY EQUATION FOR MATRIX PRODUCT STATES

Suppose a MPS satisfies the following equation:

$$|\psi(g_0-\xi)\rangle = \mathbb{R}\cdot|\psi(g_0+\xi)\rangle, \quad \text{for any} \quad \xi, \tag{1}$$

with $\mathbb{R}$ as a unitary operator, then it is easy to prove that for any operator that commutes with $\mathbb{R}$, its average value would be symmetrical with respect to g_0. In addition, as measures of quantum entanglement keep unchanged under a unitary transformation, they would also be symmetrical with respect to g_0. We will call g_0 the symmetry point of the MPS in this paper. In fact, to the best of our knowledge, all the MPSs that show the symmetry property satisfy this equation; thus, we think the equation has captured the essence of this phenomenon. We will call Eq. (1) the symmetry equation in this paper.

Suppose an operator F commutes with $\mathbb{R}$, with its average value $F(g)$ symmetrical with respect to g_0. In the vicinity of g_0, the left and right derivatives of $F(g)$ are the opposite of each other: $\frac{\partial F(g)}{\partial g}|_{g\to g_0^-}=-\frac{\partial F(g)}{\partial g}|_{g\to g_0^+}$, then $\frac{\partial F(g)}{\partial g}$ is discontinuous at $g=g_0$ if only $\frac{\partial F(g)}{\partial g}|_{g\to g_0^-}\neq 0$.[16] That explains why the symmetry point is just the singular point in many systems. For concise representations, we will not distinguish between the symmetry point and singular point in the following.

A sufficient but not necessary condition of the symmetry equation can be expressed as follows: point $g=g_0$ would be a symmetry point of the MPS, if there exist an invertible transform matrix S and a unitary matrix R satisfying

$$SA_i(g_0-\xi)S^{-1}=\sum_j R_{ij}A_j(g_0+\xi), \quad \text{with} \quad i,j=1,\ldots,d. \tag{2}$$

The unitary operator $\mathbb{R}$ of a N-particle system can be expressed as $\mathbb{R}=R^{\otimes N}$. It should be mentioned that Eq. (2) can be generalized easily to dimerized MPSs.[17] In addition, Eq. (2) works very well in most cases, while for a three-body interaction MPS (Ref. 2) and a q-deformed spin-1 MPS,[14] the symmetry points cannot be solved by Eq. (2). Fortunately, by figuring out the wave functions of finite-N chains, one can easily check that Eq. (1) still holds with $\mathbb{R}$ diagonal and its diagonal elements ± 1. Note that Eq. (2) is not a necessary condition of Eq. (1).

III. PATHS OF MPS-QPTS

In this section, we investigate two MPS examples, with $\mathbb{R}=\mathbb{I}$ and $\mathbb{R}\neq\mathbb{I}$, respectively, and map out the corresponding paths in phase diagrams. One will find that the different behaviors between MPS-QPTs and traditional QPTs can be well understood by considering the paths of the states. We will use the notation $\mathbb{I}$ for the identity matrix, $\sigma_i(i=x,y,z)$ for the Pauli matrices and $\sigma_\pm$ the Pauli raising and lowering operators in the following paper.

Example 1. The simplest case is $\mathbb{R}=\mathbb{I}$. We consider a spin-1 MPS $\{A_0,A_{+1},A_{-1}\}$ with $A_0=\mathbb{I}$, $A_{+1}=-g\sigma_+$, and $A_{-1}=g\sigma_-$, where 0 and ± 1 are the three eigenvalues of the spin-1 operator S_z.[4] Its parent Hamiltonian has been used to describe a large class of antiferromagnetic spin-1 chains,[18] with the excitation spectrum gapped (the Haldane phase) for $g>0$ and gapless at $g=0$. In addition, the string order parameter has a nonzero expectation value for $g>0$ and becomes zero at $g=0$, and the correlation length is found to be $\ln|(1+g^2)/(1-g^2)|$, which diverges at $g=0$. Thus, $g_c=0$ is indeed the critical point of the model. In addition, the longitudinal two-site correlation function is symmetrical with respect to $g_c=0$. In order to understand this symmetry behavior, we examine our conjecture $|\psi(g_0-\xi)\rangle=\mathbb{R}\cdot|\psi(g_0+\xi)\rangle$ by solving Eq. (2). We find $R=\mathbb{I}$, $S_{12}=S_{21}=0$, and $S_{11}/S_{22}=(g_0-\xi)/(g_0+\xi)=(g_0+\xi)/(g_0-\xi)$. As it holds for any ξ, we get $g_0=0$,[19] which is just the critical point g_c of the system. The invertible transform matrix is found to be $S=\begin{pmatrix}-1&0\\0&1\end{pmatrix}$. As $|\psi(g_0-\xi)\rangle=|\psi(g_0+\xi)\rangle$, the physical picture of the QPT can be illustrated as follows [see Fig. 1(b1) (top)]. For simplicity, suppose the corresponding phase space involves two phases denoted as $\wp$ and $\aleph$. The system resides in phase $\wp$ when $g<g_0$ and evolves along a path $\widehat{AC}$, which is comprised of all the quantum states a MPS describes, as g increases. When $g\to g_0^-$, the system approaches point C, which is the very boundary point between phase $\wp$ and phase $\aleph$, and it explains why the correlation length diverges at $g=g_0$. Because of the symmetry of $\psi(g)$, when $g>g_0$ the system evolves backward into phase $\wp$ along the same path $\widehat{CA}$. During the evolution $A\to C\to A$, it is obvious that all the observables should be symmetrical with respect to $g=g_0$.

Example 2. We consider a model with $\mathbb{R}\neq\mathbb{I}$. The MPS matrices are given by $A_\uparrow=\begin{pmatrix}1&g\\1&1\end{pmatrix}$ and $A_\downarrow=\begin{pmatrix}1&-g\\-1&1\end{pmatrix}$, with $\uparrow$ and $\downarrow$ related to the two eigenstates of the spin-$\frac{1}{2}$ operator S_z.[6] The state has a very interesting property: all the pairs of spins are equally entangled with each other, making it a good candidate for engineering long-range entanglement in experimentally realizable arrays of qubits or spin systems. The magnetization in the x direction is symmetrical with respect to the critical point $g_c=g_0=0$. The symmetry point, which is also the QPT point of the system, can be identified by solving Eq. (2). We find choosing two different matrix product matrices $A_\leftarrow:=(A_\uparrow+A_\downarrow)$ and $A_\rightarrow:=(A_\uparrow-A_\downarrow)$, which correspond to the two eigenstates of the spin-$\frac{1}{2}$ operator S_x, will simplify the calculations. The solution is found to be $g_0=0$ and $R=\sigma_x$. Consider its parent Hamiltonian[6]

$$H(g)=-\sum_{i=1}^{N}\frac{1}{2}(1-g)^2\sigma_{y,i}\sigma_{y,i+1}+\frac{1}{2}(1+g)^2\sigma_{z,i}\sigma_{z,i+1}+(1-g^2)\sigma_{x,i}.$$

It is apparent that $H(g_0-\xi)$ and $H(g_0+\xi)$ with $g_0=0$ describe the same quantum system in different coordinates. They can be transformed into each other by local $\pi/2$ rotations of spins around the x axis ($\sigma_{z,i}\rightleftharpoons\sigma_{y,i}$), which is consistent with the symmetry equation ($\mathbb{R}=\sigma_x^{\otimes N}$). As $[\mathbb{R},S_x]=0$, the magnetization in the x direction is symmetrical.

For a general unitary matrix $\mathbb{R}$, wave functions at the two sides of the symmetry point differ from each other by a unitary transformation and it seems as if they are just two observations for the same physical object in two different coordinate systems. One can see that in the phase diagram only paths satisfying the symmetry equation can be taken by the MPS to show a QPT, which is quite different from a traditional QPT. For a three-body interaction model,[2] it has been found that a phase transition at the triple point in the phase diagram can be described by a MPS with $A_1=\begin{pmatrix}0&0\\1&1\end{pmatrix}$ and $A_2=\begin{pmatrix}1&g\\0&0\end{pmatrix}$, thus Wolf *et al.* conclude that MPS-QPT can occur at the triple point of conventional QPT. One can check that this model satisfies the symmetry Eq. (1) with $\mathbb{R}$ being a diagonal matrix with diagonal elements ±1. We argue that the existence of a triple point in the phase diagram is neither a sufficient nor a necessary condition to show a MPS-QPT and the essence of a MPS-QPT is the existence of a special path connecting the two phases. Moreover, with the symmetry equation, one will find it is easy to understand the different analysis properties of the energy between a traditional QPT and a MPS-QPT. We consider a system with two phases shown in Fig. 1. First, by choosing appropriate energy base point, one can always scale the energy in phase $\wp$ to be zero, with the energy in phase $\aleph$ generally nonzero. When the system crosses the phase boundary through a *normal* path, for example, a path perpendicular to the boundary, a singularity is prone to be observed, and a traditional QPT happens [see Fig. 1(a)]. For a MPS-QPT, there are two cases. One is the system just reaches the phase boundary and goes backward into phase $\wp$ and never crosses into other phases, then the singularity of the energy cannot be observed [see Fig. 1(b1)]. The other is there exists a *special* path connecting the two phases [see Fig. 1(c1)], which guarantees the system be able to cross the boundary with energy invariant.

IV. TURNING POINT AND PHASE BOUNDARY POINT

In each example in Sec. III, the MPS-QPT happens at the phase boundary point C. In this section, we will give a clear physical picture that a MPS-QPT can derive from the phase boundary.

First, we consider a parametrization procedure $g:=g(x)=x^2+1$ to simulate the path $\widehat{AC}$ of the MPS in example 1. For mathematical reasons, it produces a nonunique parametrization of the phase diagram; thus, the resulting MPS seems to be trivial, however, we will show that this trivial model will be helpful to draw an intuitive picture of the next nontrivial MPS-QPT (in example 3). The new path is shown in Fig. 1(b2) (top). By solving Eq. (2) the symmetry point is found to be $x_0=0$ corresponding to a phase point B in path $\widehat{AC}$. In addition, as $g=x^2+1\geq1$, the boundary point on the end of the path $\widehat{AC}$ cannot be reached any more. Then, as x varies, the ground state of the system moves from A to B when $x\to x_0$ and then goes backward to A, with B the turning point in the path, and never reaches the boundary point C. One can see that the MPS shows a (trivial) symmetry point which has no association with the phase boundary point C at all. This kind of symmetry point is more likely to be observed in a MPS with a small D. Because, when D is small, the matrices $\{A_j\}$ can describe only a very small section in phase space, thus its path leading to the critical point could be cut off easily in different parametrization procedures. See the following nontrivial model with $\mathbb{R}\neq\mathbb{I}$.

Example 3. Consider a spin ladder model which has rotational symmetry in the x-y plane of spin space.[5] In each rung of the ladder we associate four matrices A_s, $A_{t_{+1}}$, A_{t_0}, and $A_{t_{-1}}$, where $|s\rangle$ is the single state and $|t_\mu\rangle$ with $\mu=+1,0,-1$ are the triplet states of the rung. $\{A_j\}$ are given by $A_s=xI$, $A_{t_{+1}}=g\sigma_+$, $A_{t_0}=y\sigma_z$, and $A_{t_{-1}}=\sigma_-$. The longitudinal correlation function, $G_x=-g^2(x^2+y^2-|g|)^{r-2}/(x^2+y^2+|g|)^r$, is symmetrical with respect to the three axes, which can also be identified easily by solving the symmetry equation. The corresponding correlation length $1/\ln(\frac{x^2+y^2+|g|}{x^2+y^2-|g|})$ diverges merely at $g_c=0$. Thus, for fixed x and y, there is only one path, characterized by parameter g, leading to the boundary point g_c, and the path may be cut off when more restrictions are imposed on $\{A_j\}$. For example, to construct a spin-$\frac{1}{2}$ ladder with full rotation symmetry,[5] one has to fix $g=-1$ and $y=1$, then the system never reaches the boundary point. However, the one-rung entropy $(S=\log_2(x^2+3)-[x^2\log_2(x^2)/(x^2+3)])$ still shows a symmetry point $x_0=0$. Furthermore, though $\frac{dS}{dx}|_{x\to x_0}=0$, we find that the second-order derivative d^2S/dx^2 diverges at the symmetry point. Thus, the MPS shows a singularity which has no correlation to the phase boundary point. The path of this model is shown in Fig. 1(c2), which can be figured out easily by just "rotating" the path in Fig. 1(b2). We should point out that similar analyticity of the derivatives is also reported in the dimerized spin liquid models,[7,16] where at the phase boundary point, the second-order derivative of the entropy diverges.

V. MULTIPLE SYMMETRY POINTS

For each model mentioned above, g_0 is the only symmetry point of the state. However, for certain MPS one may find a physical observable has several symmetry points. An image is drawn in Fig. 1(b3) (bottom), in which one global symmetry point and two local symmetry points are shown.

Consider parametrization procedure $g:=g(x)=x^2-1$ to simulate the path $\widehat{AC}$ in example 1. Though it is another trivial model, we find that it can help to understand the multiple symmetry point in a q-deformed spin-1 MPS. The corresponding new path is drawn in Fig. 1(b3) (top). The QPT point C can be reached twice as x varies ($x_c=\pm 1$) and the solution of the symmetry equation is found to be $x_0=0$ corresponding to point B in the path $\widehat{AC}$. Now as x varies from certain negative value to $x_c=-1$, the entire path $\widehat{AC}$ has been covered. When x varies from $x_c=-1$ to $x_0=0$, the system goes from point C to the symmetry point B. Then it moves from B to the critical point C again when x varies from $x_0=0$ to $x_c=+1$. Finally, it moves to its starting point A from the critical point C when x increases from +1. One can see that during the evolution $\widehat{AC}\to B\to\widehat{CA}$, there are three symmetry points: one is the global symmetry point $x_0=0$ and the other two are the local symmetry points $x_c=\pm 1$, which correspond to the three turning points in the path. Though the multiple symmetry point in this trivial MPS is due to mathematical reasons, one can check that the ground state of a q-deformed spin-1 chain[14] evolves similarly to Fig. 1(b3), with $\mathbb{R}\neq\mathbb{I}$, and shows three symmetry points. In order to get an intuitive image of its path, one just needs to "rotate" the path in (b3). In a complex matrix product system, such as a MPS with a larger dimension D and more free parameters, the path can be very intricate, then some points in the path may be crossed many times and more interesting behaviors may be observed.

VI. CONCLUSION

In summary, a symmetry behavior of MPS-QPTs is observed: certain physical observables are found to be symmetrical with respect to the MPS-QPT point. A symmetry equation is proposed. With the equation, we draw clear physical pictures of MPS-QPTs, and the symmetry behavior and the special analyticity of the ground-state energy of a MPS are explained. Moreover, one can figure out the QPT point of a MPS by solving the equation, without any requirement of calculating the transfer matrix or density matrix of the system. The equation acts as a selection rule for the path of a MPS-QPT. Whether there exist other selection rules for the path of a MPS-QPT needs further investigations. However, the simplest condition to ensure the system is able to cross the phase boundary with energy invariant is just the symmetry equation proposed; that is why the symmetry equation can be used in many MPS models. Furthermore, the discontinuity of the derivative of an observable is related directly to the turning point in the path, rather than the phase boundary point, though the two are in accordance with each other in many models.

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[15] In this paper, in order to give a clear physical picture of a MPS-QPT, we usually draw its path in a "phase diagram." The boundary in the phase diagram is associated with traditional QPTs. Note there is no concept of phase diagrams associated with MPS-QPTs usually.

[16] In many cases one uses $\frac{\partial F(g)}{\partial g} \neq 0$ to identify a singular point. However, in some models, even if $\frac{\partial F(g)}{\partial g}=0$, a higher-order derivative of $F(g)$ may show a singularity. An example is shown in Ref. 7. For the spin liquid model discussed in Ref. 7, the MPS has a free parameter u. At $u=0$, the spontaneous dimerization disappears and the gap between the singlet and triplet vanishes; thus, $u=0$ is indeed a phase boundary point. The single-rung entanglement $S(u)=1/u^2+3[(u^2+3)\log_2(u^2+3)-u^2\log_2(u^2)]$ is symmetrical with respect to $u=0$. In addition, it is found that $\frac{\partial S(u)}{\partial u}=0$ and $\frac{\partial^2 S(u)}{\partial u^2}$ diverges, thus the QPT is still identified by the second-order derivative of the entropy.

[17] In this paper, we only consider translationally invariant states, by taking the matrices to be site independent. An example of dimerized MPS is shown in Ref. 7.

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[19] For simplicity, the case $g\rightarrow\infty$ is not considered in this paper, which can be investigated with $g := g(x)=\frac{1}{x}$.