Quantum Phase Transitions in Matrix Product Systems

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We investigate quantum phase transitions (QPTs) in spin chain systems characterized by local Hamiltonians with matrix product ground states. We show how to theoretically engineer such QPT points between states with predetermined properties. While some of the characteristics of these transitions are familiar, like the appearance of singularities in the thermodynamic limit, diverging correlation length, and vanishing energy gap, others differ from the standard paradigm: In particular, the ground state energy remains analytic, and the entanglement entropy of a half-chain stays finite. Examples demonstrate that these kinds of transitions can occur at the triple point of ''conventional'' QPTs.

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A considerable part of modern condensed matter physics is devoted to the study of matter near zero temperature. In particular, zero-temperature quantum phase transitions (QPTs) [1], as observed in cuprate high-temperature superconductors and heavy fermion materials, have attracted enormous attention. Although an adaptation of the classical Landau-Ginzburg theory successfully describes some of these phase transitions, it is manifest that this concept is in general too narrow to cover all the fascinating aspects of the quantum world [2]. A complete and rigorous quantum mechanical description is, however, burdened by the notorious complexity of quantum correlations in highly entangled many-body systems.

The fields of condensed matter and quantum information theory study the behavior of quantum many-body systems by using complementary methodologies. Whereas the typical starting point in condensed matter theory is a Hamiltonian, from which states emerge as ground states (GSs) or excitations, quantum information theory deals primarily with quantum states, from which corresponding Hamiltonians may be constructed. For spin chains this point of view can be traced back to the seminal works on the Affleck-Kennedy-Lieb-Tasaki (AKLT) model [3] and finitely correlated states [4], and it has recently been successfully resumed in various works on matrix product states (MPSs) [5]. This led to new powerful numerical algorithms [6–8] accompanied by a better understanding of their efficiency [9], and new insights in renormalization group transformations [10] and sequential quantum generators [11].

Here we investigate QPTs in systems represented by MPSs by following the quantum information approach. Our work generalizes the findings of [4,12], which already indicated the possibility of such transitions in MPS systems, in quasiexactly solvable models. We show how to engineer QPT points between phases whose correlations or symmetries we choose *a priori*. The corresponding orders can be of local type and/or of a more subtle hidden nonlocal character. The main observation behind is that, for the systems under consideration, a singularity in a $(\mathcal{D}-1)$-dimensional transfer operator leads to a QPT in the corresponding $\mathcal{D}$-dimensional quantum system. Although these findings hold for arbitrary $\mathcal{D}$, we focus on $\mathcal{D}=1$, where a general discussion is possible on full analytic grounds.

In fact, *every state*, in particular, every GS, of a finite system can be represented as a MPS [4,6]. The power of this representation—and with it the power of density matrix renormalization group (DMRG)—stems from the fact that in many cases a low-dimensional MPS already leads to a very good approximation of the state [9]. From such a low-dimensional MPS one can in turn construct a parent Hamiltonian from which it arises as an *exact* GS. We will study the dependence of correlation functions of such systems on a smoothly varying parameter g and show that singularities can appear, reminiscent to those arising in known examples of QPTs. They appear only in the thermodynamic limit and are accompanied by diverging correlation lengths and vanishing energy gaps.

Some of the derived properties of MPS QPTs do, however, hardly fit within the conventional picture of QPTs in $\mathcal{D}=1$ spin systems: (i) At the QPT point $g=g_c$, the GS energy density e_0 is analytic (Fig. 1). (ii) The entropy of a half-chain remains finite as $g\to g_c$, which reflects the fact that MPS QPTs cannot be described in terms of conformal field theory. In fact, a lot of attention has recently been devoted to the *entanglement entropy* [13,14], resulting in the observation that the crossing of a QPT point typically coincides with the divergence of this entropy. The discussion below, however, shows that this is not the case for MPS QPTs in $\mathcal{D}=1$. (iii) Although the breaking of a discrete symmetry can be engineered, MPS QPTs can occur without spontaneous symmetry breaking since for $g\neq g_c$ the GS is typically unique.

A remark on the notion of (quantum) ''phase transitions'' is in order. In many textbooks a nonanalyticity in the GS energy density e_0 is used as the defining property of a QPT [1]. An alternative definition [15] follows the *ex-*

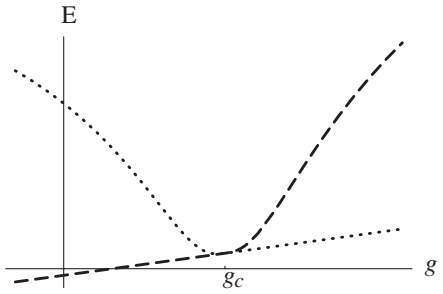

FIG. 1. Energies for the ground and first excited state as a function of g. In contrast to other QPTs the GS energy of a MPS Hamiltonian remains (by construction) analytic at the QPT point $g = g_c$. Nevertheless, the spectral gap vanishes and the correlation length diverges. Moreover, the nonanalytic change of the GS at g_c is reflected by an observable nonanalyticity of certain local expectation values.

perimental signature of phase transitions—observable discontinuities, e.g., in local observables or correlation functions. In many cases these two definitions coincide [15]; however, MPS QPTs are phase transitions only according to the second definition.

Singularities in MPSs.—Consider a MPS which is up to normalization given by

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

where $\{A_i\}$ is a set of d $D\times D$ matrices, d is the Hilbert space dimension corresponding to one site in the chain, and D is the dimension of the bonds, when we think of the state in the valence-bond picture. The state in Eq. (1) is translational invariant on a ring of length N; it has reflection symmetry if $A_i = A_i^T$, permutation symmetry if $[A_i, A_j] = 0$, and time reversal symmetry if the A_i's are real. Also other local symmetries [e.g., $SU(2)$, $\mathbb{Z}_2$] can be enforced by imposing appropriate constraints on the A_i's [4,16].

In the following we will consider systems where the matrices A_i depend on a single real parameter g. It is important to note that if the A_i depend on g in an analytic or continuous way, then so will its parent Hamiltonian constructed below. Correlation functions for m consecutive sites are given by

$$\langle S_1\cdots S_m\rangle = \frac{\mathrm{tr}[E_{\mathbb{1}}^{N-m}E_{S_1}\cdots E_{S_m}]}{\mathrm{tr}[E_{\mathbb{1}}^{N}]}, \qquad (2)$$

$$E_S = \sum_{i,j=1}^{d}\langle i|S|j\rangle A_j\otimes\bar{A}_i. \qquad (3)$$

Here S_i is any observable acting on the ith site and the bar denotes complex conjugation. For simplicity, we will focus on the generic case where the *transfer operator* $E_{\mathbb{1}}$ is diagonalizable and nondegenerate for $g \neq g_c$. Taking the thermodynamic limit ($N\to\infty$) only the right $|r\rangle$ and left $|l\rangle$ eigenvectors of $E_{\mathbb{1}}$'s largest eigenvalue ν_1 survive in Eq. (2). With the normalization $\langle l|r\rangle = 1$ this leads to

$$\langle S_1\cdots S_m\rangle = \langle l|E_{S_1}\cdots E_{S_m}|r\rangle/\nu_1^m. \qquad (4)$$

Hence, if for some $g = g_c$ there is a level crossing in the largest eigenvalues of $E_{\mathbb{1}}$, then there will typically be a discontinuity in the correlation functions (or their derivatives), even though the A_i's and with them the E's are analytic in g. Needless to say, the same argumentation holds for every observable with finite support.

A trivial example showing that discontinuities of any order n are possible is given by ($D = d = 2$)

$$A_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1+g \end{pmatrix}, \qquad A_2 = \begin{pmatrix} g^n & 0 \\ 0 & 0 \end{pmatrix}. \qquad (5)$$

Here, all derivatives $\partial_g^k\langle S_iS_{i+1}\rangle$ of order $k<n$ will be continuous at $g = g_c = 0$, whereas the nth order derivative, e.g., of $\langle\sigma^x\rangle$ turns out to be discontinuous.

Let us now discuss the properties of a general MPS in the vicinity of a transition point g_c. The decay of two-point correlations $\langle S_iS_{i+l}\rangle$ can be obtained from Eq. (2) by setting $E_{S_2} = \cdots = E_{S_{m-1}} = E_{\mathbb{1}}$ with $m = l+1$ and exploiting the Jordan decomposition of the transfer operator. This leads to

$$\langle S_iS_{i+l}\rangle - \langle S_i\rangle\langle S_{i+l}\rangle \sim \left|\frac{\nu_2}{\nu_1}\right|^{l-1}, \qquad (6)$$

where ν_2 is the second largest eigenvalue of the transfer operator. As the coupling strength approaches its QPT point value, $g\to g_c$, we get $|\nu_2|\to|\nu_1|$. Then, the correlation length $\xi = 1/\ln|\nu_1/\nu_2|$ diverges and one typically obtains long-range correlations at the transition point (see example 1 below). Note that despite the diverging correlation length there is no power-law decay at the transition point as $E_{\mathbb{1}}^{l-1}$ can give rise only to correlations which decay exponentially in l or are asymptotically constant (this can be different for $\mathcal{D}>1$ or $D=\infty$ [17]).

Since a lot of attention has recently been devoted to the relation between criticality and the scaling of the entanglement entropy [13], we give now an explicit formula for the latter. In fact, in recent works QPT points seem to be intimately connected with a logarithmic diverging behavior of the entropy of a block of consecutive spins when considered as a function of the block size. However, this is not the case for the class of QPTs discussed in the present work. The entropy of an asymptotically large block of a MPS can be calculated exactly by exploiting the freedom in the A_i's to fix the gauge $\sum_i A_iA_i^\dagger = \mathbb{1}$, $\sum_i A_i^\dagger\varrho A_i = \varrho$, where ϱ is a density matrix acting on $\mathbb{C}^D$. By the renormalization group arguments of [4,10] the spectrum of a large block converges to the spectrum of $\varrho^{\otimes 2}$ such that the entropy becomes $2S(\varrho) = -2\,\mathrm{tr}\varrho\log_2\varrho$. In particular, the entropy never exceeds $2\log D$, irrespective of how close the system is to a QPT point. This immediately implies that states exhibiting a diverging growth of the entanglement entropy cannot be described by MPSs with finite D. Moreover, following [18], the absence of a logarithmic divergence (and algebraic correlations) implies that MPS

QPTs cannot be described in terms of conformal field theory.

Higher dimensions.—Note that in the above $\mathcal{D} = 1$ case the QPT is traced back to a level crossing in the operator $E_{\mathbb{1}}$, which acts only on a single site, i.e., in dimension $\mathcal{D} - 1$. However, if the transfer operator itself has a spatial substructure, we are led to a QPT in a higher dimensional system. To be more specific, consider a $\mathcal{D}$-dimensional cubic lattice of size $N_1 \times \cdots \times N_{\mathcal{D}}$ with periodic boundary conditions. A generalization of (1), the so-called *projected entangled pair state* (PEPS) [19], is then obtained by replacing the bilinear forms A_i by tensors of order $2\mathcal{D}$, i.e., $A_i:(\mathbb{C}^D)^{\otimes 2\mathcal{D}} \to \mathbb{C}$ and the matrix product by a tensor contraction according to the edges of the lattice. As we can interpret the $\mathcal{D}$-dimensional lattice as a chain of $\mathcal{D} - 1$ dimensional systems we can introduce a transfer operator $E'_{\mathbb{1}}$ for this *chain* by contracting all $\prod_{i=2}^{\mathcal{D}} N_i$ operators $E_{\mathbb{1}}$ on a $\mathcal{D} - 1$-dimensional sublattice. In this way we are back to the one-dimensional scenario described above with the difference that the problem of calculating the largest eigenvalue of $E'_{\mathbb{1}}$ has to be tackled numerically (e.g., by DMRG or PEPS algorithms). Particular instances of such transitions were discussed in [20], where power-law decaying correlations could be determined using Monte Carlo methods. Note that by construction all *critical* GSs obtained in this way obey an *area law* for the entanglement entropy [14]. A method for deriving analytic results for particular higher dimensional instances is provided in [17].

The Hamiltonians.—Following the works on the AKLT model and finitely correlated states one can always construct a local Hamiltonian such that a given MPS is its GS: since the reduced state density operator ρ_k corresponding to k sites of a MPS has at most rank D^2, it has a null-space whenever $k > \log D^2 / \log d$. 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

$$H = \sum_i \tau_i(P_k), \tag{7}$$

with P_k being the projector onto the null-space of ρ_k and τ_i its translation to site i. By construction the GS energy is always zero; i.e., it is evidently analytic in g.

Let us now see in which cases H depends analytically on g and, moreover, is such that $|\psi\rangle$ is its unique GS for $g \neq g_c$. Consider to this end the operator

$$R = \mathcal{A}^{\otimes k}(\mathbb{1}_D \otimes \omega^{\otimes(k-1)} \otimes \mathbb{1}_D)\mathcal{A}^{\dagger\otimes k}, \tag{8}$$

where $\omega = \sum_{i,j=1}^{D} |ii\rangle\langle jj|$ and $\mathcal{A}|\alpha, \beta\rangle = \sum_i [A_i]_{\alpha,\beta}|i\rangle$. Note that, if A_i depends analytically on g, R also depends analytically on g. It is evident from the valence-bond construction of the MPS that, in general, $\text{range}(\rho_k) \subseteq \text{range}(R)$. However, if both eigenvectors $|r\rangle$ and $|l\rangle$ have full Schmidt rank, then a straightforward calculation shows that $\text{range}(\rho_k) = \text{range}(R)$. Hence, if this Schmidt rank condition is satisfied on both sides of g_c (which is generically the case), then $H(g)$ indeed depends smoothly on g.

It was proven in [4,16] that the GS of Hamiltonians of the form (7) is unique if the largest eigenvalue of $E_{\mathbb{1}}$ is nondegenerate (i.e., $g \neq g_c$), $\text{rank}(\rho_k) = D^2$, and

$$\text{range}\,(\rho_k) \otimes \mathbb{C}^d \cap \mathbb{C}^d \otimes \text{range}(\rho_k) = \text{range}(\rho_{k+1}). \tag{9}$$

It is also shown there that the latter condition is always satisfied if we replace k by $k + 1$, i.e., take $H = \sum_i \tau_i(P_{k+1})$.

The analyticity of H together with the uniqueness of its GS for $g \neq g_c$ immediately imply that a nonanalyticity in the expectation values can only be caused by a vanishing energy gap at g_c. Note that a degeneracy in the GS is equivalent to a degeneracy in $E_{\mathbb{1}}$. This means that there is no spontaneous symmetry breaking in one of the phases, unless $|\nu_1| = |\nu_2|$ for an entire interval (e.g., for $g \geq g_c$). However, for a degenerate $E_{\mathbb{1}}$ arbitrary broken discrete symmetries are possible [16].

Examples.—We will now consider some examples in more detail. By imposing constraints on the matrices A_i, we can thereby *engineer* systems having desired properties (symmetries, orders, discrete symmetry breaking, etc.).

Example 1: Three-body interactions. We start by considering the case $D = d = 2$, i.e., A_1, A_2 being two-by-two matrices. By the arguments above every such state has a parent Hamiltonian with local three-body interactions. In fact, many of these Hamiltonians are similar to ones which appear or can be realized in optical lattices [21]. We construct an example with $\mathbb{Z}_2$ symmetry by imposing the existence of a similarity transformation which interchanges A_1 and A_2, i.e., $X^{-1}A_1X = A_2$ and $X^{-1}A_2X = A_1$. This is indeed the case if we choose

$$A_1 = \begin{pmatrix} 0 & 0 \\ 1 & 1 \end{pmatrix}, \quad A_2 = \begin{pmatrix} 1 & g \\ 0 & 0 \end{pmatrix}, \quad \text{and} \quad X = \begin{pmatrix} 0 & g \\ 1 & 0 \end{pmatrix}.$$

The corresponding transfer operator $E_{\mathbb{1}}$ has largest eigenvalues $1 \pm g$ leading to a singularity at $g = g_c = 0$. A straightforward calculation shows a discontinuity in the first derivative of $\langle \sigma_i^\alpha \sigma_{i+1}^\alpha \rangle (\alpha = x, y, z)$, whereas all two-point expectation values are continuous. Moreover, the magnetization in the x direction can serve as a signature of the phase transition, although it is not an order parameter in the usual sense since there is no corresponding broken symmetry. Whereas for $g > 0$ we have $\langle \sigma^x \rangle = 4g/(1 + g)^2$, it vanishes for $g < 0$.

At the QPT point g_c the state is a Greenberger-Horne-Zeilinger (GHZ) state; i.e., two-point correlations become independent of the distance. For $g = -1$ it is equal to the *cluster state* [22], and for $g = 1$ all spins point in the x direction. The parent Hamiltonian is $\mathbb{Z}_2$ symmetric:

$$H = \sum_i 2(g^2 - 1)\sigma_i^z \sigma_{i+1}^z - (1 + g)^2 \sigma_i^x, \tag{10}$$

$$+ (g - 1)^2 \sigma_i^z \sigma_{i+1}^x \sigma_{i+2}^z. \tag{11}$$

Hence, it is a combination of an Ising interaction with transverse magnetic field (10) and a cluster state Hamiltonian (11). Since a constant term was omitted, the GS energy density is $e_0 = -2(1 + g^2)$, and one can readily check condition (9) implying that the GS is indeed unique for $g \neq g_c = 0$. The above Hamiltonian can be embedded into a two-parameter family, which is up to a global factor of $2(1 + g^2)$,

$$H(\gamma, h) = -\sum_i \frac{1+\gamma}{2}\sigma_i^x - \frac{1-\gamma}{2}\sigma_{i-1}^z\sigma_i^x\sigma_{i+1}^z + h\sigma_i^z\sigma_{i+1}^z,$$

and can be mapped onto a system of noninteracting Fermions by a Jordan-Wigner transformation. Moreover, $H(\gamma, h)$ can be mapped onto the XY model via a Kramers-Wannier duality transformation [23]. This in turn exhibits second order QPTs on the lines $h = \pm 1$ and $\gamma = 0$ for $h \in (-1, 1)$. The path parametrized by g is given by $\gamma^2 + h^2 = 1$ (the *disorder line* in the XY model). Hence, the MPS transition occurs at the triple point of "conventional" QPTs exhibiting algebraically decaying correlations, diverging entanglement entropies [23], and satisfying both QPT definitions.

Example 2: Two-body interactions. The previous example corresponded to the case of a *local* order parameter. We now discuss an example with nonlocal *string order*. To this end, consider $D = 2$, $d = 3$, i.e., states of a spin-1 chain which are GSs of nearest-neighbor interactions. The most popular MPS in this class is certainly the GS of the spin-1 AKLT model, which exhibits a hidden (string) order. In fact, this state can be embedded into a one-parameter family with MPS QPT. If we choose $\{A_i\} = \{-\sigma_z, \sigma^-, g\sigma^+\}$, then $E_{\mathbb{1}}$ has eigenvalues -1 and $1 \pm g$ leading to a diverging correlation length for $g \to g_c = 0$. Moreover, the first derivative of $\langle S^z\rangle$ has a discontinuity at $g_c = 0$, where $\langle S^z\rangle \to 1$, i.e., the state becomes ferromagnetic. For $g = \pm 2$ we get AKLT states, which merely differ by local unitary transformations. For $g \to \pm\infty$ the GS becomes the Néel GHZ state $(|\uparrow\downarrow\uparrow\cdots\rangle + |\downarrow\uparrow\downarrow\cdots\rangle)/\sqrt{2}$. As already shown in [4] (with a different parametrization for $g < 0$), the corresponding Hamiltonian is rotationally symmetric in the XY plane, gapped with nondegenerate GS (unless $g = g_c$), and has the form

$$H = \sum_i (2 + g^2)\vec{S}_i\vec{S}_{i+1} + 2(\vec{S}_i\vec{S}_{i+1})^2 + 2(4 - g^2)(S_i^z)^2 - (g + 2)^2(S_i^zS_{i+1}^z)^2 + g(g + 2)\{S_i^zS_{i+1}^z, \vec{S}_i\vec{S}_{i+1}\}_+. \quad (12)$$

Conclusion.—MPSs provide a convenient playground for investigating novel types of quantum phase transitions that do not fit in the traditional framework. We provided various examples of such QPTs and it is easy to construct many more: given two predetermined MPS and associated parent Hamiltonians, choose an interpolation between the two. If on the chosen path the transfer operator exhibits a level crossing in the largest eigenvalue, then the system undergoes a QPT. MPS QPTs may serve as a clarifying theoretical test bed and as an alternative model for the description of QPTs with atypical properties (which might be realized in optical lattices [21]).

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