

Quantum fidelity and quantum phase transitions in matrix product states

Marco Cozzini,^{1,2} Radu Ionicioiu,^{2,*} and Paolo Zanardi^{2,3}

¹*Dipartimento di Fisica, Politecnico di Torino, Corso Duca degli Abruzzi 24, I-10129 Torino, Italy*

²*Quantum Information Group, Institute for Scientific Interchange (ISI), Viale Settimio Severo 65, I-10133 Torino, Italy*

³*Department of Physics and Astronomy, University of Southern California, Los Angeles, California 90089-0484, USA*

(Received 30 November 2006; revised manuscript received 19 July 2007; published 19 September 2007)

Matrix product states, a key ingredient of numerical algorithms widely employed in the simulation of quantum spin chains, provide an intriguing tool for quantum phase transition engineering. At critical values of the control parameters on which their constituent matrices depend, singularities in the expectation values of certain observables can appear, in spite of the analyticity of the ground state energy. For this class of generalized quantum phase transitions, we test the validity of the recently introduced fidelity approach, where the overlap modulus of ground states corresponding to slightly different parameters is considered. We discuss several examples, successfully identifying all the present transitions. We also study the finite size scaling of fidelity derivatives, pointing out its relevance in extracting critical exponents.

DOI: [10.1103/PhysRevB.76.104420](https://doi.org/10.1103/PhysRevB.76.104420)

PACS number(s): 05.30.-d, 64.60.-i

I. INTRODUCTION

The study of many-body quantum systems is at the same time a fascinating and challenging field of research. This is due to the richness of inherently complex phenomena arising in the presence of a large number of interacting particles, among which quantum phase transitions (QPTs) occupy a distinguished position. These transitions take place at zero temperature and are driven by an external parameter, such as, for example, the magnetic field in superconductors.

Recently, it has been shown that the quantum fidelity—the overlap modulus—of two finite size ground states corresponding to neighboring control parameters is a good indicator of QPTs. Indeed, the fidelity in a finite size system undergoing a QPT in the thermodynamic limit (TDL) typically drops abruptly at critical points, as a consequence of the dramatic state transformation involved in a transition. This yields a finite size precursor of the transition, whose effectiveness has been tested in various contexts where the ground state can be calculated exactly, either analytically or numerically. These include the Dicke model, the one-dimensional XY model in a transverse field, and general quadratic fermionic Hamiltonians.^{1,2} The ground state fidelity has also been analyzed by Zhou and Barjaktarevič with emphasis on renormalization group transformations.³

In the present paper, we further pursue this approach by analyzing QPTs in systems described by matrix product states (MPSs).^{4–6} These states are at the basis of efficient numerical methods used in the analysis of spin chain systems, such as the density matrix renormalization group (DMRG) algorithm. When considered dependent on a control parameter g , they can give rise to *generalized* QPTs, i.e., transitions where some observable quantity presents a nonanalytic behavior in spite of the regularity of the ground state energy.⁷ We show that the quantum fidelity of two neighboring (in terms of g) MPSs is an effective tool not only in detecting the critical point g_c but also in giving the correct scaling at g_c . The success of the fidelity approach in analyzing MPS-QPTs further proves the generality of the procedure, which, as stressed in Refs. 1 and 2, does not re-

quire any *a priori* understanding of the structure (order parameter, correlation functions, topology, etc.) of the considered system. It is also worth pointing out that this method seems to have some advantage with respect to other quantum information based techniques. For example, quantum phase transitions in MPSs do not give rise to the logarithmic divergence of the entropy of block entanglement observed in other systems,⁸ thereby ruling out this quantity as a reliable transition indicator. On the other hand, other entanglement measures can be used, e.g., single site entanglement and concurrence, whose derivatives often provide interesting information about criticality.⁹ We discuss the results obtained by these methods in one of the simple examples we analyze below. As it will be shown, also these latter measures turn out to be less effective than the fidelity approach.

In the following, we will first present a derivation of the overlap formula for general MPSs (Sec. II), discussing some general features of these systems, and then study in detail the MPS examples introduced in Ref. 7 (Sec. III). As in Refs. 1 and 2, the analysis will be carried out also in terms of fidelity derivatives, which are the most suitable tool to observe finite size scaling properties. In particular, we will explicitly show how to extract the critical exponent of the correlation length from these quantities (Sec. III A), thus demonstrating the independence and the completeness of our approach. Finally, we will report on the entanglement analysis in Sec. III B.

II. FIDELITY FOR MATRIX PRODUCT STATES

Suppose we have a closed spin chain with N sites. Let d be the dimension of the Hilbert space at each site. The matrix product states are defined as⁶

$$|g\rangle := |\psi(g)\rangle = \frac{1}{\sqrt{\mathcal{N}}} \sum_{i_1, \dots, i_N=0}^{d-1} \text{Tr}(A_{i_1} \cdots A_{i_N}) |i_1 \cdots i_N\rangle, \quad (1)$$

where the A_j 's, with $j=0, \dots, d-1$, are $D \times D$ matrices, D is the dimension of the bonds in the so-called valence bond picture, and $\mathcal{N} := \sum_{i_1, \dots, i_N=0}^{d-1} |\text{Tr}(A_{i_1} \cdots A_{i_N})|^2$ is a normalization factor. The valence bond picture is inspired by the valence

bond solid states introduced by⁴ Affleck, Kennedy, Lieb, and Tasaki (AKLT). Within this approach, MPSs are obtained by starting from a virtual system made of two D -dimensional spins for each site of the real chain of d -dimensional spins. These virtual spins are coupled in pairs in such a way that each of the two spins at a given site is linked by a valence bond to one of the two spins at a neighboring site. The valence bond basically means that these spin pairs are in a maximally entangled state. In practice, one has a one-to-one correspondence between the virtual links and the sites of the real spin chain. MPSs are finally obtained by suitably projecting the virtual chain onto the desired spin chain, where the projector coefficients give rise to the A_j matrices above.

It turns out that every state can be represented as a MPS provided the dimension D of its constituent matrices is sufficiently large.¹⁰ However, the main importance of MPSs stems from the fact that relevant classes of one-dimensional physical states can be very well approximated by MPSs with low-dimensional matrices. In practice, when speaking of MPSs, one implicitly refers to this case. This effectiveness of the MPS description is at the basis of the success of the DMRG algorithm, which can be seen as a variational procedure within the MPS space.⁶

Since our goal is to explore quantum phase transitions in such states, we assume that the matrices $A_j = A_j(g)$ depend on one or more parameters, generically denoted by g . The overlap of two MPSs corresponding to different g 's is

$$\langle g_1 | g_2 \rangle = [\mathcal{N}(g_1)\mathcal{N}(g_2)]^{-1/2} \times \sum_{\mathbf{i} \in \mathcal{I}_d^N} \text{Tr}[A_{i_1}^*(g_1) \cdots A_{i_N}^*(g_1)] \text{Tr}[A_{i_1}(g_2) \cdots A_{i_N}(g_2)], \quad (2)$$

where $\mathbf{i} = (i_1, \dots, i_N)$. In order to simplify the formulas, we will work with the unnormalized overlap

$$F(g_1, g_2) := \sqrt{\mathcal{N}(g_1)\mathcal{N}(g_2)} \langle g_1 | g_2 \rangle, \quad (3)$$

and we obviously have $\mathcal{N}(g_a) = F(g_a, g_a)$, $a = 1, 2$. Using the identity $\text{Tr}(A)\text{Tr}(B) = \text{Tr}(A \otimes B)$, the overlap can be computed exactly for MPSs³ and we obtain

$$F(g_1, g_2) = \text{Tr}[E^N(g_1, g_2)] = \sum_{k=1}^{D^2} \lambda_k^N(g_1, g_2), \quad (4)$$

where λ_k are the eigenvalues of the $D^2 \times D^2$ matrix

$$E(g_1, g_2) := \sum_{i=0}^{d-1} A_i^*(g_1) \otimes A_i(g_2). \quad (5)$$

The latter is the generalization of the transfer operator $E_1(g) := E(g, g)$, which we assume to be diagonalizable with eigenvalues $\lambda_k(g) := \lambda_k(g, g)$. Also, since $A \otimes B$ and $B \otimes A$ are isospectral, one has $F(g_1, g_2) = F(g_2, g_1)^*$.

The main object of our study will be the fidelity of two neighboring states,

$$\mathcal{F}(g; \delta) := |\langle g - \delta | g + \delta \rangle| = \frac{|F(g - \delta, g + \delta)|}{\sqrt{\mathcal{N}(g - \delta)\mathcal{N}(g + \delta)}}, \quad (6)$$

for a small variation δ in the parameter space spanned by g . Defined this way, the fidelity depends not only on the parameter g driving the QPT but also on its variation δ . Expanding the fidelity in δ , we obtain $\mathcal{F}(g; \delta) \approx 1 + \delta^2 \mathcal{F}(g; \delta)|_{\delta=0} \delta^2 / 2$ [since $\mathcal{F}(g; \delta)$ reaches its maximum for $\delta=0$, the first derivative vanishes]. Thus, the rate of change of the fidelity close to a critical point is given by the second derivative¹¹ of the fidelity^{1,2}

$$S(g) := \delta_{\delta}^2 \mathcal{F}(g; \delta)|_{\delta=0}, \quad (7)$$

and this is the relevant quantity we will study to determine the scaling at the critical point $g = g_c$. Note that $S(g)$ is connected to the ground state variation $|\psi'(g)\rangle = \delta_g |\psi(g)\rangle$. For example, for real states one has the simple second order expansion $\mathcal{F}(g; \delta) \approx 1 - 2\delta^2 \|\psi'(g)\|^2$. The general expression of the second derivative has the form¹²

$$S(g) = -4 \delta_{g_1} \delta_{g_2} \ln F(g_1, g_2)|_{g_1=g_2=g}. \quad (8)$$

Indeed, from $\mathcal{F}(g; 0) = 1$ and $\delta_{\delta} \mathcal{F}(g; \delta)|_{\delta=0} = 0$, one has $\delta_{\delta}^2 \ln \mathcal{F}(g; \delta)|_{\delta=0} = \delta_{\delta}^2 \mathcal{F}(g; \delta)|_{\delta=0} = S(g)$ and then

$$S(g) = \frac{1}{2} \delta_{\delta}^2 \ln \frac{F(g - \delta, g + \delta) F(g + \delta, g - \delta)}{F(g - \delta, g - \delta) F(g + \delta, g + \delta)} \Big|_{\delta=0} = (\delta_g^2 - \delta_g^2) \ln F(g - \delta, g + \delta)|_{\delta=0}, \quad (9)$$

from which Eq. (8) follows immediately.

The general behavior of the fidelity for matrix product states in the thermodynamic limit can be inferred from Eq. (4). Without loss of generality we can assume the eigenvalues λ_k of the generalized transfer operator E to be ordered $|\lambda_1| \geq |\lambda_2| \geq \dots \geq |\lambda_{D^2}|$. Then, $F(g_1, g_2) = \sum_{k=1}^{D^2} \lambda_k^N(g_1, g_2) = \lambda_1^N [1 + \sum_{k=2}^{D^2} (\lambda_k/\lambda_1)^N]$ and, provided $|\lambda_1| > |\lambda_k|$ for $k = 2, \dots, D^2$, in the thermodynamic limit $N \rightarrow \infty$, one finds $F(g_1, g_2) \sim \lambda_1^N$. Since the same holds for the normalization factors $\mathcal{N}(g) = F(g, g)$, whenever the maximum eigenvalues λ_1 are nondegenerate, the large N behavior of the fidelity must be of the form $\mathcal{F}(g; \delta) \sim \alpha^N$, with $0 \leq \alpha \leq 1$ by construction. Typically, $\alpha \neq 1$ and the fidelity decays exponentially in the TDL.³ If $E_1(g)$ exhibits a level crossing in the largest eigenvalue for a critical coupling g_c , the degeneracy $|\lambda_1(g_c)| = |\lambda_2(g_c)|$ gives rise to a discontinuity of some expectation values in the TDL (called a generalized QPT in Ref. 7). In this case, the previous discussion has to be modified in order to include all the degenerate eigenvalues. In general, the vanishing of the fidelity is typically strongly enhanced at critical points.

A similar analysis can be done for the second derivative $S(g)$ of the fidelity. When a single eigenvalue λ_1 dominates, in the TDL one can replace F with λ_1^N in Eq. (8), thereby recovering the expected² linear scaling $\propto N$:

$$S(g) \sim -4N \delta_{g_1} \delta_{g_2} \ln \lambda_1(g_1, g_2)|_{g_1=g_2=g}. \quad (10)$$

In contrast, at the critical point two or more eigenvalues of $E(g_1, g_2)$ are equal in modulus. For example, at $g = g_c$ one

can have $|\lambda_1(g_c)|=|\lambda_2(g_c)|>|\lambda_k(g_c)|$ for $k>2$. Then, in the TDL

$$\begin{aligned}
 S(g_c) &\sim \lim_{g \rightarrow g_c} -4\partial_{g_1}\partial_{g_2} \ln(\lambda_1^N + \lambda_2^N)|_{g_1=g_2=g} \\
 &= \lim_{g \rightarrow g_c} \left\{ -N^2 \frac{4\lambda_1^N \lambda_2^N}{(\lambda_1^N + \lambda_2^N)^2} \partial_{g_1} \ln \frac{\lambda_1}{\lambda_2} \partial_{g_2} \ln \frac{\lambda_1}{\lambda_2} \right. \\
 &\quad \left. -4N \sum_{k=1}^2 \frac{\lambda_k^N}{\lambda_1^N + \lambda_2^N} \partial_{g_1} \partial_{g_2} \ln \lambda_k \right\} \Bigg|_{g_1=g_2=g}, \quad (11)
 \end{aligned}$$

where $\lambda_{1,2}=\lambda_{1,2}(g_1, g_2)$. Hence, at the transition one typically recovers the divergence $S(g_c) \propto N^2$ already observed in Ref. 2. We also note that by defining $\theta := \ln(\lambda_1/\lambda_2)$, the term in the second line of Eq. (11) can be rewritten in the compact form $[N|\partial_{g_1}\theta/\cosh(N\theta/2)|]^2$. This follows from the equality $\partial_{g_1} \ln(\lambda_1/\lambda_2) \partial_{g_2} \ln(\lambda_1/\lambda_2) = |\partial_{g_1} \ln(\lambda_1/\lambda_2)|^2$, due to the relation $\lambda_{1,2}(g_2, g_1) = \lambda_{1,2}^*(g_1, g_2)$. Then, it is clear that this term vanishes for $N \rightarrow \infty$ unless $\Re\theta=0$, i.e., $|\lambda_1| = |\lambda_2|$. In the latter case, instead, assuming $\partial_{g_1}\theta$ to be finite, the scaling $\propto N^2$ is evident. Finally, we point out that the limit $g \rightarrow g_c$ in Eq. (11) is necessary to deal with possible singularities in the derivatives of the λ_k 's at the transition (see the examples below).

Before entering the analysis of practical cases, let us comment about the relationship between a given MPS and the Hamiltonian of which the MPS is the ground state. In the above discussion, we have related the occurrence of QPTs with singularities in the properties of the state under consideration. However, the study of QPTs is usually concerned with the properties of the Hamiltonian and, in particular, with the behavior of its energy spectrum. In this respect, two remarks are in order. First of all, given any MPS $|g\rangle$ it is possible under suitable conditions to construct a local parent Hamiltonian $H(g)$ whose unique ground state is exactly the considered MPS and whose ground state energy identically vanishes for any g (see, for example, Ref. 6). It is then clear that the aforementioned generalized QPTs cannot be detected by looking at singularities of the ground state energy derivatives. Second, focusing on the ground state itself rather than on the Hamiltonian, besides being a natural point of view within the MPS description, is also a natural consequence of the fidelity framework. This approach to QPTs, indeed, is clearly based on the study of the state transformation under the variation of the coupling parameter.

III. EXAMPLES

In the following, we are going to study the explicit examples of MPSs described in Ref. 7. Without loss of generality, we assume $g_1 = g - \delta < g_2 = g + \delta$.

A. Fidelity and second order matrix product state quantum phase transitions

Example 1. Take $D=2$, $d=3$, and $\{A_j\} = \{-Z, \sigma_-, g\sigma_+\}$; in the following, we will use the notation X, Z for the Pauli matrices, σ_{\pm} being the corresponding raising and lowering operators. This one-parameter family of MPSs contains the

ground state of spin-1 AKLT model for $g = \pm 2$ and has a critical point at $g_c=0$ (see Ref. 7). The model is also significant because it has nonlocal string order. The parent Hamiltonian with two-body interaction is given by

$$\begin{aligned}
 H = \sum_i &[(2+g^2)\mathbf{S}_i \cdot \mathbf{S}_{i+1} + 2(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 + 2(4-g^2)(S_i^z)^2 \\
 &+ (g+2)^2(S_i^z S_{i+1}^z)^2 + g(g+2)\{\mathbf{S}_i^z \mathbf{S}_{i+1}^z, \mathbf{S}_i \cdot \mathbf{S}_{i+1}\}], \quad (12)
 \end{aligned}$$

where \mathbf{S}_i is the spin operator acting on the i th site. The eigenvalues of the transfer operator $E = Z \otimes Z + \sigma_- \otimes \sigma_- + g_1 g_2 \sigma_+ \otimes \sigma_+$ are $(-1, -1, 1 \pm \sqrt{g_1 g_2})$ and Eq. (4) yields

$$F(g_1, g_2) = (1 + \sqrt{g_1 g_2})^N + (1 - \sqrt{g_1 g_2})^N + 2(-1)^N \quad (13)$$

and $\mathcal{N}(g) = F(g, g) = (1+g)^N + (1-g)^N + 2(-1)^N$.

Let us analyze the behavior of the fidelity $\mathcal{F}(g; \delta)$ defined in Eq. (6). Since $\mathcal{F}(g; \delta)$ is evidently symmetric in both g and δ , we can safely assume $g \geq 0$, $\delta > 0$. Three cases can then be distinguished, according to the behavior of the eigenvalues of the transfer operators:

(i) $g > \delta$, where $\mathcal{F}(g; \delta) \sim \alpha^N$ for $N \gg 1$, with $\alpha = (1 + \sqrt{g^2 - \delta^2}) / \sqrt{(1+g-\delta)(1+g+\delta)} < 1$;

(ii) $g = \delta$, where $\mathcal{F}(g; \delta) \sim a/(1+2\delta)^{N/2}$ for $N \gg 1$, with $a=2$ for N even and $a=2\delta\sqrt{N(N-1)}$ for N odd [this is the case where the largest eigenvalue of $E(g-\delta, g+\delta)$ is degenerate and the decaying behavior of the fidelity is slightly modified]; and

(iii) $g < \delta$, where two of the eigenvalues of $E(g_1, g_2)$ are complex and, for $N \gg 1$, the fidelity exhibits an oscillatory behavior driven by $|\cos(N\varphi_0)|$, $\varphi_0 = \arctan \sqrt{\delta^2 - g^2}$, with a decaying envelope given by $2\alpha^N$, $\alpha = \sqrt{(1+\delta^2-g^2)/[(1+\delta-g)(1+\delta+g)]} < 1$. Explicitly, at the critical point $g = g_c = 0$ the overlap becomes

$$\langle -\delta | \delta \rangle = \frac{(1+\delta^2)^{N/2} \cos(N\varphi_0) + (-1)^N}{[(1+\delta)^N + (1-\delta)^N]/2 + (-1)^N}, \quad (14)$$

where $\varphi_0 = \arctan \delta$. Then, $\mathcal{F}(0; \delta) = |\langle -\delta | \delta \rangle|$ (note that the overlap can be negative at this point).

The fidelity behavior in the neighborhood of the critical point is shown in Fig. 1 for $\delta = 10^{-3}$ and various values of N . It is evident that although for a fixed δ the fidelity vanishes in the TDL for any g , the rate of decrease is much faster at the transition. This fidelity drop provides a useful finite size precursor of the quantum phase transition taking place in the infinite system. In the inset of the figure, we zoom on the oscillatory behavior in the interval $g \in (-\delta, \delta)$, where states on different sides of the transition are considered. Note that oscillations start to be visible only for $N\varphi > \pi$, i.e., $N > N_{\text{osc}}$, $N_{\text{osc}} = \pi / \arctan \sqrt{\delta^2 - g^2}$, which for $g=0$ and $\delta \ll 1$ reduces to $N_{\text{osc}} \sim \pi / \delta$.

The second derivative $S(g)$ of the fidelity can be calculated analytically using formula (8). We find

$$S(g \neq 0) \sim -\frac{N}{|g|(1+|g|)^2}, \quad (15)$$

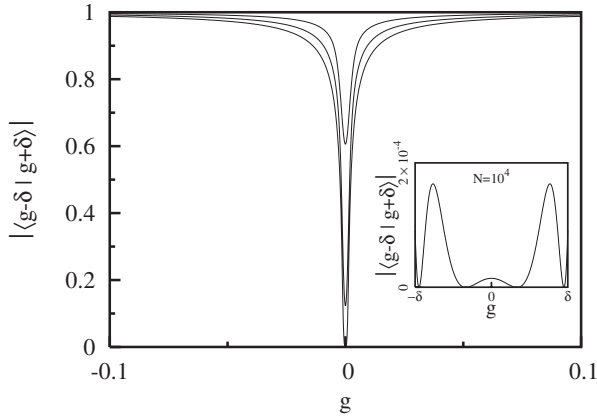


FIG. 1. Fidelity $\mathcal{F}(g; \delta) = |\langle g - \delta | g + \delta \rangle|$ as a function of g for Example 1 with $\delta = 10^{-3}$ and $N = 1000, 2000$, and 3000 . Inset: Close to the critical point, the fidelity oscillates for states belonging to different phases ($\delta = 10^{-3}$, $N = 10^4$).

$$S(g=0) = \begin{cases} -N(N-1) & (N \text{ even}) \\ -(N-2)(N-3)/3 & (N \text{ odd}), \end{cases} \quad (16)$$

where Eq. (15) corresponds to Eq. (10) and gives the asymptotic behavior for large N , while Eq. (16) is exact. As in Ref. 2, the critical point is identified by a divergence $\propto N^2$ of the second derivative $S(g)$ of the fidelity.

In Fig. 2, we plot $\log_{10}|S(g)|$ for different values of N . In the inset of the figure, the curves are plotted in rescaled units, giving rise to data collapsing (lines for different values of N are practically indistinguishable in the inset, merging into a single thick line). This shows that $S(g)/N^2$ is basically a function of gN only. This is reminiscent of the usual scaling behavior of diverging expectation values in second order quantum phase transitions. Indeed, if the quantity P in a one-dimensional system diverges algebraically in the TDL for some critical coupling g_c , i.e., $P_\infty \sim c_\infty |g - g_c|^{-\rho}$, the finite

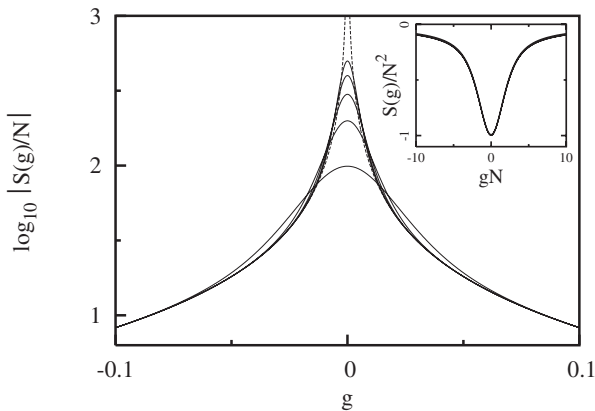


FIG. 2. Finite size scaling for $S(g)$. The second derivative $S(g)$ is plotted for $N = 100, 200, \dots, 500$ (logarithm is base 10). The peak at $g=0$ scales with N accordingly to Eq. (16). The dashed line corresponds to the asymptotic behavior given by Eq. (15). The inset shows the data collapsing for the same curves ($N = 100, 200, \dots, 500$) when plotted in rescaled units.

size scaling ansatz in the critical region reads $P_N = N^{\rho/\nu} Q(N|g - g_c|^\nu)$, where ν is the critical exponent of the bulk correlation length ξ_c and Q is some function.¹³ This is due to the fact that at criticality, once properly rescaled by some power of the size of the system, the value of P is expected to depend only on the dimensionless ratio L/ξ_c between the system size $L \propto N$ and the correlation length. Since the latter diverges at the transition like $\xi_c \propto 1/|g - g_c|^\nu$, one immediately finds $L/\xi_c \propto N|g - g_c|^\nu$. In our case, $P_N = S/N = NQ(N|g|)$ with $g_c = 0$, so that we obtain $\rho = \nu = 1$. The result $\rho = 1$ agrees with Eq. (15), which, for $g \rightarrow 0$, yields $P_\infty \sim -|g|^{-1}$. The value of ν can instead be checked by explicitly calculating the correlation length. For example, for S^x the correlation length defined by $\langle S_i^x S_{i+l}^x \rangle - \langle S_i^x \rangle \langle S_{i+l}^x \rangle \propto e^{-l/\xi_c}$ is given in the TDL by the standard formula $\xi_c = 1/\ln|\lambda_1/\lambda_2|$ (see, e.g., Ref. 7), where λ_1 (λ_2) is the eigenvalue of $E_1(g)$ with the (second) largest modulus. In our case, $|\lambda_1| = 1 + |g|$ and $|\lambda_2| = 1$, so that $\xi_c = 1/\ln(1 + |g|) \sim 1/|g|$, i.e., $\nu = 1$ and the finite size scaling estimate is confirmed.¹⁴

The next examples of this section correspond to three-body interaction Hamiltonians, again taken from Ref. 7. Qualitatively, they all feature the same behavior as Example 1: in the asymptotic limit, $|S(g)|/N$ diverges proportionally to $1/|g|$ at the critical point $g_c = 0$, while the peak height of $S(g=0)$ scales with N^2 .

Example 2. Consider $D = d = 2$ and $A_0 = (1 - Z)/2 + \sigma_-$, $A_1 = (1 + Z)/2 + g\sigma_+$. The three-body Hamiltonian is \mathbb{Z}_2 symmetric and has a critical point at $g_c = 0$, where the state is a Greenberger-Horne-Zeilinger (GHZ) state, and reads

$$H = \sum_i 2(g^2 - 1)Z_i Z_{i+1} - (1 + g)^2 X_i + (g - 1)^2 Z_i X_{i+1} Z_{i+2}. \quad (17)$$

The generalized transfer operator $E(g_1, g_2)$ has eigenvalues $(0, 0, 1 \pm \sqrt{g_1 g_2})$, very similar to Example 1. The function $F(g - \delta, g + \delta)$ is then still symmetric in g and δ .

Since the largest eigenvalue λ_1 is the same as in Example 1, the TDL behavior of $\mathcal{F}(g, \delta)$ and $S(g)$ is unchanged. However, the parity dependent term $(-1)^N$ is now absent. Then, the asymptotic behavior of $S(g \neq 0)$ is still given by Eq. (15), while the parity dependence of Eq. (16) is lost and one simply has $S(g=0) = -2N(N-1)$. The latter result follows from Eq. (11), which applies exactly to this case even for finite N . Indeed, here only two eigenvalues of $E(g_1, g_2)$ are different from zero and one has the level crossing $\lambda_1(g=0) = \lambda_2(g=0)$. Note that due to the divergence of the double derivative $\partial_{g_1} \partial_{g_2} \ln \lambda_{1,2}$ calculated in $g_1 = g_2 = 0$, also the term in the last line of Eq. (11) gives rise to a contribution $\propto N^2$, in spite of its apparent linearity in N for $|\lambda_1| = |\lambda_2|$. This explains the necessity of the limit $g \rightarrow g_c$ in Eq. (11).

Example 3. Consider $A_0 = X$, $A_1 = \sqrt{g(1-Z)}/2$. The eigenvalues of $E(g_1, g_2)$ are $(\pm 1, (\sqrt{g_1 g_2} \pm \sqrt{g_1 g_2 + 4})/2)$. As before, the scaling of the system can be seen from the behavior of $S(g)$ in the thermodynamic limit, driven by $\lambda_1(g_1, g_2) = (\sqrt{g_1 g_2} + \sqrt{g_1 g_2 + 4})/2$. We find

$$S(g \neq 0) \sim -\frac{4N}{|g|(g^2+4)^{3/2}}, \quad (18)$$

$$S(g=0) = \begin{cases} -N^2/4 & (N \text{ even}) \\ -(N^2-1)/6 & (N \text{ odd}), \end{cases} \quad (19)$$

where Eq. (18) gives the large N behavior. The parity dependence of Eq. (19) is caused by the negative eigenvalues of $E(g_1, g_2)$, giving rise to terms oscillating like $(-1)^N$.

Example 4. Take $A_0 = \sigma_+$, $A_1 = \sigma_- + \sqrt{g}(1+Z)/2$. This MPS is the ground state of the following Hamiltonian:

$$H = -\sum_i g(X_i + X_i Z_{i+1} + Z_i X_{i+1} + Z_i X_{i+1} Z_{i+2}) + (1+2g^2)Z_i - 2Z_i Z_{i+1} - Z_i Z_{i+1} Z_{i+2}. \quad (20)$$

The eigenvalues of $E(g_1, g_2)$ are $(0, 0, (\sqrt{g_1 g_2} \pm \sqrt{g_1 g_2 + 4})/2)$. Hence, the asymptotic behavior of $S(g)$ is again given by Eq. (18), while $S(0) = -N^2/2$ for N even and $S(0) = -(N^2-1)/6$ for N odd. Parity dependence arises from $(\sqrt{g_1 g_2} - \sqrt{g_1 g_2 + 4})/2 = -1$ for $g_1 = g_2 = 0$.

B. Fidelity, concurrence, and single site entanglement

While all the above examples fit in the same picture, which is typical of the second order quantum phase transitions already studied in Refs. 1 and 2, the next example, albeit trivial as matrix product state, features a different behavior, which will serve as a basis for some additional comments on the fidelity approach to QPTs.

Example 5. Take $D = d = 2$, $A_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1+g \end{pmatrix}$, $A_1 = \begin{pmatrix} g^n & 0 \\ 0 & 0 \end{pmatrix}$. The matrix $E(g_1, g_2)$ has the eigenvalues $1+g_1$, $1+g_2$, $(1+g_1)(1+g_2)$, and $1+g_1^n g_2^n$. As discussed in Sec. II, QPTs take place when two or more eigenvalues of $E_1(g) = E(g, g)$ share the largest modulus. We then have to compare $1+g$, $(1+g)^2$, and $1+g^{2n}$. Clearly, for $g < 0$ one has $\lambda_1(g) = 1+g^{2n}$, while for $g \geq 0$ the dominant eigenvalue is determined by the ratio $r(g) := (1+g^{2n})/(1+g)^2$. The equation $r(g) = 1$ can be rewritten as $g(g^{2n-1} - g - 2) = 0$. Apart from the trivial solution $g_c = 0$, for $n \geq 2$ a second solution $g'_c > 1$ exists, so that in the region $0 \leq g \leq g'_c$ one has $\lambda_1(g) = (1+g)^2$, while for $g > g'_c$ one obtains again $\lambda_1(g) = 1+g^{2n}$. For $n=1$, the point g'_c can be considered at infinity and the latter level crossing never occurs.

In order to evaluate the fidelity, we have to substitute the above eigenvalues in Eq. (6). For simplicity, here we restrict our analysis to the fidelity of ground states belonging to the same phase, avoiding the discussion of the effects shown in the inset of Fig. 1 for Example 1. In the phase corresponding to the interval $g \in (0, g'_c)$, where $\lambda_1(g) = (1+g)^2$, one has $\lambda_1(g_1, g_2) = (1+g-\delta)(1+g+\delta)$. The normalized fidelity in the TDL then results $\mathcal{F}(g; \delta) \sim [(1+g-\delta)(1+g+\delta)/\sqrt{(1+g-\delta)^2(1+g+\delta)^2}]^N = 1$, so that one has a constant phase in this region, due to the factorization of the largest eigenvalue of $E(g-\delta, g+\delta)$. Outside this region, such a factorization is absent and the fidelity vanishes exponentially with the size of the system.

The asymptotic behavior of the second derivative $S(g)$ can be calculated accordingly. In the interval $g \in (0, g'_c)$,

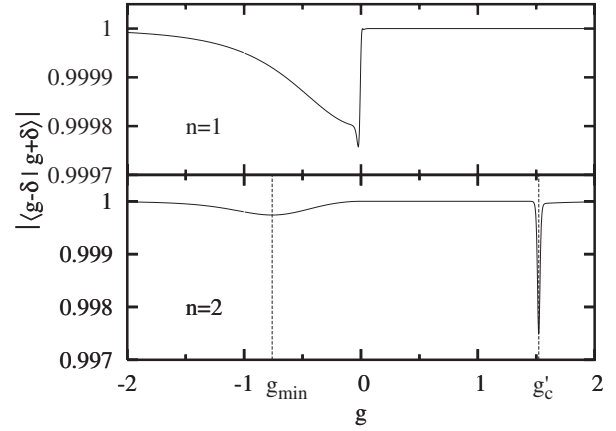


FIG. 3. Fidelity for the model given in Example 5, with $\delta = 10^{-3}$ and $N=100$; $n=1$ (top) and $n=2$ (bottom).

where the eigenvalue $(1+g)^2$ dominates, one finds $S(g)=0$ in the TDL, while for $g \notin [0, g'_c]$, where the leading eigenvalue is given by $1+g^{2n}$, Eq. (10) yields the formula

$$S(g) \sim -4Nn^2 g^{2n-2}/(1+g^{2n})^2. \quad (21)$$

The latter function, which is evidently symmetric in g , has a minimum at $g_{\min} = -[(n-1)/(n+1)]^{1/2n}$ [since $|g_{\min}| < g'_c$, the minimum position for $g > 0$ is instead given by g'_c itself, as $S(g)$ increases monotonically for $g > g'_c$]. Note that, while $S(g)$ is continuous at $g = g_c = 0$, where $S(0) = 0$, at the second critical point $g = g'_c$ one has the discontinuity $\lim_{g \rightarrow (g'_c)^-} S(g) = 0 \neq \lim_{g \rightarrow (g'_c)^+} S(g) = -4Nn^2(g'_c + 2)/[g'_c(1+g'_c)^4]$, where the latter result is obtained by substituting the defining relation $r(g'_c) = 1$ into Eq. (21). Furthermore, exactly at the critical point g'_c one has the superextensive scaling $S(g'_c) \sim -N^2[2n - 1 + (n-1)g'_c]^2/(1+g'_c)^4$.

The finite size behavior of the fidelity is shown in Fig. 3 for $N=100$ and $\delta=10^{-3}$. Due to the approximated relation $\mathcal{F}(g; \delta) \approx 1 + S(g)\delta^2/2$, one can here recognize also the scaling of $S(g)$. In particular, in the lower panel where the case $n=2$ is plotted, the minimum at g_{\min} and the superextensive scaling at $g'_c(n=2) \approx 1.521$ are evident.

For this simple example, it is also possible to find a compact analytic expression for the ground state $|g\rangle$. Due to the commutativity $[A_0, A_1] = 0$, one has $\sqrt{N}|g\rangle = \sum_{\mathbf{i} \in \mathbb{Z}_2^N} \text{Tr}(A_0^{N-k} A_1^k) |i_1 \cdots i_N\rangle$ with $k = \sum_{j=1}^N i_j$. Then, by using $\text{Tr}(A_0^N) = 1 + (1+g)^N$ and $\text{Tr}(A_0^{N-k} A_1^k) = g^{nk}$ for $k \neq 0$, one finds

$$\begin{aligned} \sqrt{N}|g\rangle &= [1 + (1+g)^N] |0\rangle^{\otimes N} + \sum_{k=1}^N g^{nk} \binom{N}{k}^{1/2} |D_N^{(k)}\rangle \\ &= (1+g)^N |0\rangle^{\otimes N} + (1+g^{2n})^{N/2} |\phi(g)\rangle^{\otimes N}, \end{aligned} \quad (22)$$

where $|D_N^{(k)}\rangle = \binom{N}{k}^{-1/2} \sum_{\mathbf{i} \in I_k} |i_1 \cdots i_N\rangle$ with $I_k = \{\mathbf{i} \in \mathbb{Z}_2^N | \sum_{j=1}^N i_j = k\}$ is a Dicke state¹⁵ and $|\phi(g)\rangle = (|0\rangle + g^n |1\rangle)/\sqrt{1+g^{2n}}$ is a normalized single site state. Since the normalization is $\mathcal{N} = \text{Tr} E_1^N$, depending on the dominating eigenvalue of E_1 three cases are possible in the TDL:

- (i) $\lambda_1(g) = (1+g)^2 > \lambda_2(g)$ and $|g\rangle \rightarrow |0\rangle^{\otimes N}$,

- (ii) $\lambda_1(g) = 1 + g^{2n} > \lambda_2(g)$ and $|g\rangle \rightarrow |\phi(g)\rangle^{\otimes N}$, and
 (iii) $\lambda_1(g) = \lambda_2(g)$ and, in the nontrivial case $g = g'_c$, one has¹⁶ $|g\rangle \rightarrow (|0\rangle^{\otimes N} + |\phi\rangle^{\otimes N})/\sqrt{2}$.

The above analysis can be summarized in the following table, where we recall the results for the largest transfer operator eigenvalue $\lambda_1(g)$ and for the large N behavior of the function $S(g)$ and the ground state $|g\rangle$:

	$g \in [0, g'_c)$	$g = g'_c$	$g \notin [0, g'_c]$
$\lambda_1(g)$	$(1+g)^2$	$1+g^{2n} = (1+g)^2$	$1+g^{2n}$
$S(g)$	0	$\propto N^2$	$\propto N$
$ g\rangle$	$ 0\rangle^{\otimes N}$	$(0\rangle^{\otimes N} + \phi(g'_c)\rangle^{\otimes N})/\sqrt{2}$	$ \phi(g)\rangle^{\otimes N}$

It is worth noting that the apparent drop of the fidelity at g_{\min} in the $g < 0$ phase for $n \geq 2$ does not correspond to a QPT. Indeed, the scaling of $S(g_{\min})$ does not present any peculiar behavior with respect to the rest of the $g < 0$ phase. On the contrary, the scaling of S changes its nature at $g=0$ and $g=g'_c$, highlighting the transitions, although in a very different way from the typical behavior observed in the previous second order QPTs. The transition at $g=0$ corresponds to a discontinuity in $\partial_g^2 \langle X \rangle$ (Ref. 7), while that at $g=g'_c$ to a discontinuity of $\langle X \rangle$ itself.¹⁷ Due to the permutation symmetry arising from the commutativity of A_0, A_1 , the correlation length cannot here be defined (the usual formula $\xi_c = 1/\ln|\lambda_1/\lambda_2|$ does not hold). In practice, the transitions of Example 5 appear to be of first order.

For this example, we also investigate concurrence and single site entanglement, mainly focusing on the critical point $g_c=0$. Of course, the fact that the state is factorized in the TDL trivially implies the vanishing of these quantities in this limit. We are, however, interested in the finite size scaling of the derivatives of these measures, in the spirit of Ref. 9. We are motivated by various aspects. First, as mentioned before, in MPS-QPTs the block entanglement entropy does not exhibit the logarithmic divergence observed in other quantum phase transitions, posing the question whether other entanglement properties usually signaling quantum criticality behave differently in this case. Second, we are interested in comparing the effectiveness of the fidelity approach against other quantum information theoretical methods. The simple nature of this example allows for a fully analytical treatment.

Concurrence. We compute the concurrence for the reduced density matrix of 2 qubits in the chain (the choice of the qubits is unimportant due to the permutation symmetry mentioned above). The density matrix of two spins $\rho^{(2)}$ is obtained by tracing the initial $\rho = |g\rangle\langle g|$ over all the other spins in the chain. By exploiting the symmetries arising from the commutation relations $[A_i, A_j] = 0$ and recalling that $\rho^{(2)} = \sum_{i,j,k,l=0}^1 \rho_{ij,kl}^{(2)} |ij\rangle\langle kl|$ is a 4×4 real symmetric matrix, one finds $\rho_{ij,kl}^{(2)} = \rho_{ji,kl}^{(2)} = \rho_{ij,lk}^{(2)}$. Together with the normalization $\text{Tr} \rho^{(2)} = 1$, this implies that only five entries of $\rho^{(2)}$ are independent, e.g., $\rho_{00,00}^{(2)}$, $\rho_{00,01}^{(2)}$, $\rho_{00,11}^{(2)}$, $\rho_{01,01}^{(2)}$, and $\rho_{01,11}^{(2)}$, significantly simplifying the calculation in the standard basis. Otherwise, one can use Eq. (22), easily obtaining

$$\rho^{(2)} = [(1+g)^{2N} |00\rangle\langle 00| + (1+g^{2n})^N |\phi\phi\rangle\langle\phi\phi| + (1+g)^N (1+g^{2n}) (|00\rangle\langle\phi\phi| + |\phi\phi\rangle\langle 00|)]/\mathcal{N}(g). \quad (23)$$

Having $\rho^{(2)}$, the concurrence for two qubits is defined as¹⁸ $C = \max\{0, \sqrt{\mu_1} - \sqrt{\mu_2} - \sqrt{\mu_3} - \sqrt{\mu_4}\}$, where μ_i 's are the eigenvalues, in decreasing order, of the operator $\rho^{(2)}(\sigma_y \otimes \sigma_y) \times (\rho^{(2)})^*(\sigma_y \otimes \sigma_y)$. We finally have

$$C(g) = \frac{2g^{2n} |(1+g)^N|}{\mathcal{N}(g)}. \quad (24)$$

In the thermodynamic limit, both $C(g)$ and its first derivative vanish, so that the kind of transition signatures found, e.g., in Ref. 9, are absent here. However, for $n=1$, the fourth derivative $\partial_g^4 C|_{g=0}$ has a divergence in the TDL; for $n \geq 2$, the singularity is present in even higher derivatives.

Single site entanglement. This quantity is the von Neumann entropy of a single spin $\mathcal{S} = -\text{Tr}(\rho^{(1)} \log_2 \rho^{(1)})$, where $\rho^{(1)}$ is the reduced density matrix of a single site. Again, from Eq. (22) one finds

$$\rho^{(1)} = [(1+g)^{2N} |0\rangle\langle 0| + (1+g^{2n})^N |\phi\rangle\langle\phi| + (1+g)^N \sqrt{1+g^{2n}} (|0\rangle\langle\phi| + |\phi\rangle\langle 0|)]/\mathcal{N}(g), \quad (25)$$

whose eigenvalues are $\lambda_{\pm} = (1 \pm \sqrt{1 - 4 \det \rho^{(1)}})/2$, with $\lambda_+ = 1 - \lambda_-$ and

$$\det \rho^{(1)} = \frac{g^{2n} (1+g)^{2N} [(1+g^{2n})^{N-1} - 1]}{\mathcal{N}^2(g)}. \quad (26)$$

The single site entanglement entropy $\mathcal{S} = -\lambda_+ \log_2 \lambda_+ - \lambda_- \log_2 \lambda_-$ vanishes in the thermodynamic limit at $g=0$, together with its first derivative. For $n=1$, one finds a divergence in $\partial_g^4 \mathcal{S}|_{g=0}$, while the divergence is shifted to higher derivatives for $n \geq 2$, similar to the concurrence. The considered divergence is, however, due to the functional form of the von Neumann entropy. Indeed, $\lambda_- \rightarrow 0$ for $g \rightarrow 0$, giving rise to a singularity in the logarithm.

We conclude this analysis by briefly discussing the TDL of these entanglement measures at the critical point $g=g'_c$, where the state is not factorized (see the table above). The single site reduced density matrix in the TDL is simply $\rho^{(1)}(g'_c) = (|0\rangle\langle 0| + |\phi\rangle\langle\phi|)/2$ and $\det \rho^{(1)}(g'_c) = [1 - 1/(1+g'_c)^2]/4$. Then, $\lambda_{\pm}(g'_c) = [1 \pm 1/(1+g'_c)]/2$ and $\mathcal{S}(g'_c) \neq 0$. Note, however, that $C(g'_c) = 0$ in the TDL, reminiscent of the behavior of the GHZ state. This can be seen from the simple TDL of Eq. (23), namely, $\rho^{(2)}(g'_c) = (|00\rangle\langle 00| + |\phi\phi\rangle\langle\phi\phi|)/2$.

IV. CONCLUSIONS

In conclusion, we have investigated the quantum fidelity of slightly different matrix product states dependent on a parameter g in the context of quantum phase transitions. For generic MPSs, the overlap can be related analytically to the eigenvalues of a generalized transfer operator, among which the largest in modulus plays a crucial role. If the latter is nondegenerate (in modulus), the fidelity typically exhibits an exponential decay in the thermodynamic limit and its second

derivative is proportional to the size N of the system. If instead more eigenvalues share the largest modulus, a quantum phase transition can take place and the fidelity second derivative $S(g)$ generally scales with N^2 . We have demonstrated this behavior in the exhaustive analysis of some simple examples, taken from Ref. 7, where possible exceptions have also been pointed out. Moreover, we have shown that the second derivative of the fidelity is a useful quantity for the quantitative analysis of the scaling properties of the system at the transition point. From the finite size scaling behavior of $S(g)$, we have indeed estimated the critical exponent for the correlation length, finding agreement with the explicit calculation. Finally, for one of the considered examples, we have analyzed both concurrence and single site entanglement. Although the latter quantities did provide signatures of the undergoing quantum phase transitions, this information was hidden in high order derivatives, making it much more difficult to extract than the fidelity (or its second derivative).

The fidelity analysis has the advantage of providing a unified framework to detect very different types of phase transitions. For the concrete examples analyzed here, singularities in the fidelity are related to level crossings in the transfer operator, recovering the known transition mechanism for matrix product states. The results presented here further contribute to demonstrate the generality of the fidelity approach to quantum phase transitions,¹⁹ supporting the findings of Refs. 1 and 2.

ACKNOWLEDGMENTS

We thank L. Amico and P. Giorda for valuable discussions and comments. We are grateful to H.-Q. Zhou and J. P. Barjaktarevič for sending us the draft of Ref. 3, which we received as a private communication before the realization of this work.

*Present address: Hewlett-Packard Laboratories, Filton Road, Stoke Gifford, Bristol BS34 8QZ, United Kingdom.

¹P. Zanardi and N. Paunković, Phys. Rev. E **74**, 031123 (2006); P. Zanardi, M. Cozzini, and P. Giorda, J. Stat. Mech.: Theory Exp. (2007) L02002.

²M. Cozzini, P. Giorda, and P. Zanardi, Phys. Rev. B **75**, 014439 (2007).

³H.-Q. Zhou and J. P. Barjaktarevič, arXiv:cond-mat/0701608 (unpublished).

⁴I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, Phys. Rev. Lett. **59**, 799 (1987); Commun. Math. Phys. **115**, 477 (1988).

⁵M. Fannes, B. Nachtergaele, and R. F. Werner, Europhys. Lett. **10**, 633 (1989); Commun. Math. Phys. **144**, 443 (1992); S. Östlund and S. Rommer, Phys. Rev. Lett. **75**, 3537 (1995); S. Rommer and S. Östlund, Phys. Rev. B **55**, 2164 (1997).

⁶D. Pérez-García, F. Verstraete, M. M. Wolf, and J. I. Cirac, Quantum Inf. Comput. **7**, 401 (2007).

⁷M. M. Wolf, G. Ortiz, F. Verstraete, and J. I. Cirac, Phys. Rev. Lett. **97**, 110403 (2006).

⁸G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. **90**, 227902 (2003); G. Refael and J. E. Moore, *ibid.* **93**, 260602 (2004); V. E. Korepin, *ibid.* **92**, 096402 (2004).

⁹A. Osterloh, L. Amico, G. Falci, and R. Fazio, Nature (London) **416**, 608 (2002).

¹⁰G. Vidal, Phys. Rev. Lett. **91**, 147902 (2003).

¹¹Note that we are calculating derivatives in the finite size system, where quantities are expected to be analytical. Later on, we will

analyze the scaling behavior and consider the TDL of the obtained expressions.

¹²Considering the fidelity $|\langle g-\delta|g+\delta\rangle|$ corresponds to taking a variation 2δ between the states. This gives rise to the factor 4 in formula (8) and differs from Refs. 1 and 2.

¹³M. E. Fisher and M. N. Barber, Phys. Rev. Lett. **28**, 1516 (1972); M. N. Barber, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, London, 1983), Vol. 8, p. 145.

¹⁴If one instead considers S^z for this particular example, the correlation length is given by $\xi_c=1/\ln|\lambda_1/\lambda_4|$, where $\lambda_4=1-g$. This is due to the vanishing of some matrix elements related to the eigenvalues $\lambda_2=\lambda_3=-1$. Nevertheless, it is easy to see that the critical exponent is still $\nu=1$.

¹⁵R. H. Dicke, Phys. Rev. **93**, 99 (1954).

¹⁶Note that $|0\rangle^{\otimes N}$ and $|\phi(g')\rangle^{\otimes N}$ become orthogonal in the TDL, in accordance with the normalization factor $1/\sqrt{2}$.

¹⁷In the limit $N\rightarrow\infty$ one has $\langle X(g)\rangle\rightarrow 0$ for $g\in[0,g']$, $\langle X(g')\rangle\rightarrow (g')^n/[1+(g')^{2n}]$, and $\langle X(g)\rangle\rightarrow 2g^n/(1+g^{2n})$ for $g\in[0,g']$. Hence, for example, $\lim_{g\rightarrow 0}\partial_g^n\langle X\rangle=2n!$, while $\lim_{g\rightarrow 0}\partial_g^n\langle X\rangle=0$.

¹⁸W. K. Wootters, Phys. Rev. Lett. **80**, 2245 (1998).

¹⁹By using Uhlmann's fidelity for mixed states, one can extend this kind of analysis to finite temperature systems and therefore even to classical phase transitions. See Ref. 3 and P. Zanardi, H.-T. Quan, X.-G. Wang, and C.-P. Sun, Phys. Rev. A **75**, 032109 (2007).