Spontaneous symmetry breaking and bifurcations in ground-state fidelity for quantum lattice systems

Jian-Hui Zhao, Hong-Lei Wang, Bo Li, and Huan-Qiang Zhou
Centre for Modern Physics and Department of Physics, Chongqing University, Chongqing 400044, People's Republic of China
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Spontaneous symmetry breaking occurs in a system when its Hamiltonian possesses a certain symmetry, whereas the ground-state wave functions do not preserve it. This provides such a scenario that a bifurcation, which breaks the symmetry, occurs when some control parameter crosses its critical value. It is unveiled that the ground-state fidelity per lattice site exhibits such a bifurcation for quantum lattice systems undergoing quantum phase transitions. The significance of this result lies in the fact that the ground-state fidelity per lattice site is *universal*, in the sense that it is model independent, in contrast to (model-dependent) order parameters. This fundamental quantity may be computed by exploiting the developed tensor network algorithms on infinite-size lattices. We illustrate the scheme in terms of the quantum Ising model in a transverse magnetic field and the spin-$\frac{1}{2}$ XYX model in an external magnetic field on an infinite-size lattice in one spatial dimension.

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I. INTRODUCTION

Quantum phase transitions (QPTs) [1,2] arise from the cooperative behaviors in quantum many-body systems, in which long-range orders emerge. In the conventional Landau-Ginzburg-Wilson paradigm, the most fundamental notion is spontaneous symmetry breaking (SSB), with the symmetry-broken phase characterized by the nonzero values of a local order parameter. An SSB occurs in a system when its Hamiltonian enjoys a certain symmetry, whereas the ground-state wave functions do not preserve it [3,4]. The implication of an SSB is twofold: first, a system has stable and degenerate ground states, each of which breaks the symmetry of the system; second, the symmetry breakdown results from random perturbations. This leads to such a scenario that a bifurcation, which breaks the symmetry, occurs, when some control parameter crosses its critical value. Conventionally, this is reflected in local order parameters.

The latest advances in our understanding of QPTs originate from the perspectives of both entanglement [5] and fidelity [6–9], which are basic notions in quantum information science. In Refs. [7,8], it has been argued that the ground-state fidelity per lattice site is *fundamental* in the sense that it may be used to characterize QPTs, regardless of what type of internal order is present in quantum many-body states. The argument is solely based on the basic postulate of quantum mechanics on quantum measurements, which implies that two nonorthogonal quantum states are not reliably distinguishable [10]. In other words, the ground-state fidelity per lattice site is able to describe QPTs arising from an SSB and/or topological order [11]. This has been further confirmed in Refs. [12,13], where topologically ordered states in the Kitaev model on the honeycomb lattice and the Kosterlitz-Thouless phase transition are investigated from the fidelity perspective, respectively. Moreover, even for systems with symmetry-breaking orders, it is advantageous to adopt the ground-state fidelity per lattice site instead of using the conventional local order parameters due to the fact that it is model independent although one may systematically derive local order parameters from tensor network (TN) representations of quantum many-body ground-state wave functions by investigating the reduced density matrices for local areas on an infinite-size lattice [14]. However, it remains unclear whether or not it is possible for the ground-state fidelity per lattice site to capture bifurcations arising from an SSB.

In this paper, we attempt to fill in this gap. First, we demonstrate that the developed TN algorithms on infinite-size lattices may produce degenerate ground states arising from an SSB, each of which results from a randomly chosen initial state subject to an imaginary time evolution. Second, it is unveiled that an SSB is reflected as a bifurcation in the ground-state fidelity per lattice site for quantum lattice systems undergoing QPTs with symmetry-breaking orders [15]. The significance of this conclusion lies in the fact that, on the one hand, this establishes the connection between the fidelity approach to QPTs and the singularity theory; on the other hand, it is of practical importance since it makes possible to locate transition points without the need to compute the derivatives of the ground-state fidelity per lattice site with respect to the control parameter [16]. In contrast, the von Neumann entropy, a bipartite entanglement measure, fails to distinguish degenerate symmetry-breaking ground states. We illustrate the general scheme in terms of the quantum Ising model in a transverse magnetic field and the spin-$\frac{1}{2}$ XYX model in an external magnetic field. Here, it is worth emphasizing that, although the scheme is applicable to quantum lattice models in any spatial dimensions, we restrict ourselves to quantum systems on an infinite-size lattice in one spatial dimension. This is achieved by exploiting the infinite matrix product state (iMPS) algorithm initiated by Vidal [17]. The extension to quantum lattice systems in two and higher spatial dimensions, which requires to use the infinite projected entangled-pair state (iPEPS) algorithm [18], is deferred to another publication [19].

II. INFINITE MATRIX PRODUCT STATE ALGORITHM AND SPONTANEOUS SYMMETRY BREAKING

For quantum many-body systems on an infinite-size lattice in one spatial dimension, Vidal [17] developed a variational algorithm to compute their ground-state wave functions based on their MPS representations, which is a variant of the MPS algorithm [20,21] on a finite-size lattice in one spatial dimension. Here, we briefly recall the key ingredients of the algorithm. Assume that the Hamiltonian is translationally invariant, and consists of the nearest-neighbor interactions: $H=\Sigma_i h^{[i,i+1]}$, with $h^{[i,i+1]}$ being the nearest-neighbor two-body Hamiltonian density. In the canonical MPS representation [17], a quantum state for a quantum many-body system on an infinite-size lattice in one spatial dimension is parametrized in terms of a three-index tensor Γ^s_{Alr} or Γ^s_{Blr} and a diagonal (singular value) matrix λ_A or λ_B. Γ^s_{Alr} or Γ^s_{Blr} is attached to each site, and λ_A or λ_B is attached to each bond, with the subscripts A and B depending on the evenness and oddness of the ith site and the i-th bond, respectively. Here, s is a physical index, $s=1,\ldots,d$, with d being the dimension of the local Hilbert space, and l and r denote the bond indices, $l,r=1,\ldots,\chi$, with χ being the truncation dimension. The ground-state wave function is projected out by performing the imaginary time evolution on an initial state $|\Psi(0)\rangle$, which amounts to computing $|\Psi(\tau)\rangle=\exp(-H\tau)|\Psi(0)\rangle / |\exp(-H\tau)|\Psi(0)\rangle|$. For large enough τ and a generic initial state $|\Psi(0)\rangle$, it yields a good approximation to the ground-state wave function, as long as there is a gap in the spectrum of the system. Following the Suzuki-Trotter decomposition [22], the imaginary time evolution operator is reduced to a product of two-site evolution operators acting on sites i and $i+1: U(i,i+1)=\exp(-h^{[i,i+1)]}\delta\tau)$, $\delta\tau \ll 1$. Notice that, acting a two-site gate $U(i,i+1)$ on a MPS representation produces two issues: first, the state is no longer in the form of a MPS; second, it breaks the translational invariance under two site shifts. The former is remedied by performing a singular value decomposition of a matrix contracted from one Γ^s_{Alr}, one Γ^s_{Blr}, one λ_A, and two λ_Bs, with only the χ largest singular values retained. This yields the new tensors Γ^s_{Alr}, Γ^s_{Blr}, and λ_A, which are used to update the tensors for all the sites, thus restoring the translational invariance under two site shifts. Repeating this procedure until the ground-state energy converges, one may generate the system's ground-state wave functions in the MPS representations.

Remarkably, for a system with symmetry-breaking orders, the iMPS algorithm automatically produces degenerate ground states arising from an SSB in the symmetry-broken phase, each of which breaks the symmetry of the system. Moreover, the symmetry breakdown results from the fact that an initial state has been chosen randomly. It is worth mentioning that, for quantum lattice systems in one spatial dimension, continuous symmetries cannot be spontaneously broken [23] due to strong quantum fluctuations [24]. Therefore, we shall restrict ourselves to the discussion of quantum lattice systems with a discrete symmetry group Z_2 [25].

III. BIFURCATIONS IN THE GROUND-STATE FIDELITY PER LATTICE SITE

Now consider a quantum many-body system, with a discrete symmetry group Z_2, on an infinite-size lattice in one spatial dimension. Assume that the system undergoes a continuous QPT with Z_2 symmetry spontaneously broken when a control parameter λ varies. According to the definition [7,8], the ground-state fidelity per lattice site, $d(\lambda_1,\lambda_2)$, is the scaling parameter, which characterizes how fast the fidelity $F(\lambda_1,\lambda_2)\equiv|\langle\Psi(\lambda_2)|\Psi(\lambda_1)\rangle|$ between two ground states $|\Psi(\lambda_1)\rangle$ and $|\Psi(\lambda_2)\rangle$ goes to zero when the thermodynamic limit is approached. In fact, the ground-state fidelity $F(\lambda_1,\lambda_2)$ asymptotically scales as $F(\lambda_1,\lambda_2)\sim d(\lambda_1,\lambda_2)^L$, with L as the number of sites in a finite-size lattice. Remarkably, the ground-state fidelity per lattice site is well defined in the thermodynamic limit and satisfies the properties inherited from the fidelity $F(\lambda_1,\lambda_2)$: (i) normalization $d(\lambda,\lambda)=1$; (ii) symmetry $d(\lambda_1,\lambda_2)=d(\lambda_2,\lambda_1)$; and (iii) range $0 \le d(\lambda_1,\lambda_2)\le 1$.

In the Z_2 symmetric phase, the ground state is nondegenerate, whereas in the Z_2 symmetry-broken phase, two degenerate ground states arise. Now let us see what this implies for the ground-state fidelity per lattice site, $d(\lambda_1,\lambda_2)$. If we choose $\Psi(\lambda_2)$ as a reference state, with λ_2 in the Z_2 symmetric phase, then the ground-state fidelity per lattice site, $d(\lambda_1,\lambda_2)$, cannot distinguish two degenerate ground states $|\Psi_\pm(\lambda_1)\rangle$ in the Z_2 symmetry-broken phase. Here, $|\Psi_+(\lambda_1)\rangle = P|\Psi_-(\lambda_1)\rangle$, with P being the operation generating the symmetry group Z_2. This follows from the fact that $\langle\Psi(\lambda_2)|\Psi_+(\lambda_1)\rangle=\langle\Psi(\lambda_2)|P|\Psi_+(\lambda_1)\rangle=\langle\Psi(\lambda_2)|\Psi_-(\lambda_1)\rangle$ for any large but finite size L. However, if we choose $\Psi(\lambda_2)$ as a reference state, with λ_2 in the Z_2 symmetry-broken phase, then $d(\lambda_1,\lambda_2)$ is able to distinguish two degenerate ground states. Therefore, for a given truncation dimension χ, a pseudo phase transition point λ_χ manifests itself as a *bifurcation point* [15]. An extrapolation to $\chi=\infty$ determines the critical point λ_c. Therefore, the pinch point, first introduced in Refs. [7,8] as an intersection of two singular lines to characterize phase transition points, is identified as a bifurcation point.

In contrast, the von Neumann entropy, a bipartite entanglement measure, fails to distinguish degenerate symmetry-breaking ground states. This is due to the fact that the von Neumann entropy is fully determined by the singular value matrices λ_A and λ_B, whereas all the information concerning an SSB is encoded in the tensors Γ^s_{Alr} and Γ^s_{Blr}.

IV. MODELS

As an illustration, let us consider two quantum systems with the symmetry group Z_2. The first is the quantum Ising model in a transverse magnetic field on an infinite-size lattice in one spatial dimension. It is described by the Hamiltonian

$$H=-\sum_{i=-\infty}^{\infty}(S_x^{[i]}S_x^{[i+1]}+\lambda S_z^{[i]}), \qquad (1)$$

where $S_\alpha^{[i]}$ $(\alpha=x,z)$ are the Pauli spin operators of the ith spin-$\frac{1}{2}$ and λ is the transverse magnetic field. The model is invariant with respect to the operation: $S_x^{[i]}\to -S_x^{[i]}$ for all the sites simultaneously, thus it enjoys the Z_2 symmetry. As is well known, it undergoes a QPT, with a critical point at $\lambda_c=1$ [26].

The second is the spin-$\frac{1}{2}$ XYX model in an external magnetic field, with the Hamiltonian

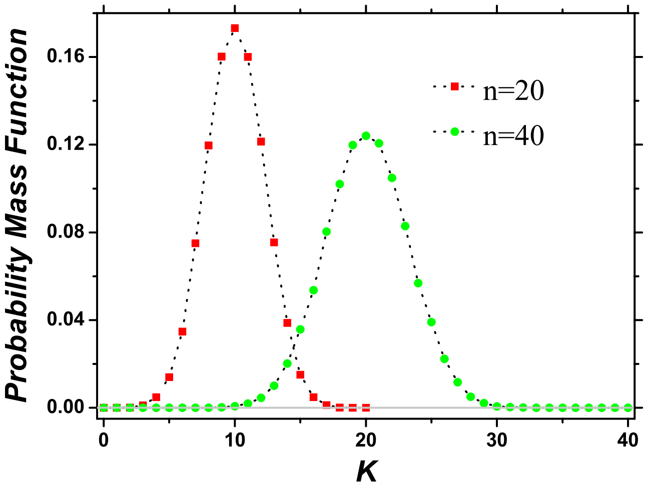

FIG. 1. (Color online) The probability mass function $\Pr(K=k)=C_n^k p^k(1-p)^{n-k}$ for the quantum Ising model in a transverse magnetic field in the Z_2 symmetry-broken phase, with $\lambda=1/2$. Here, n is the total number of the trials to be observed simultaneously, and $k(=0,1,2,\ldots,n)$ is the number of getting positive values of the order parameter $\langle S_x^{[i]}\rangle$, and $C_n^k=n!/[k!(n-k)!]$ is the binomial coefficient. By a trial we mean that the order parameter $\langle S_x^{[i]}\rangle$ for a ground-state wave function arising from a random chosen initial state is measured.

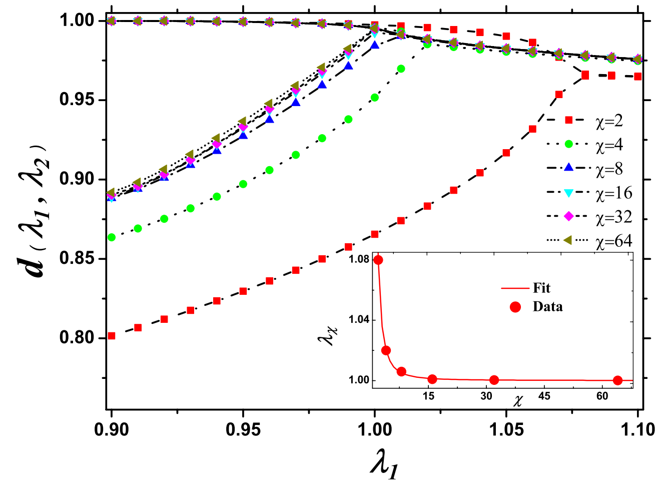

FIG. 2. (Color online) Main: the ground-state fidelity per lattice site, $d(\lambda_1,\lambda_2)$, as a function of the transverse magnetic field strength λ_1, with a fixed λ_2, for the quantum Ising model in a transverse field. We have chosen here $\lambda_2=0.9$. Inset: the critical point is determined from an extrapolation of the pseudo phase transition point λ_χ for the truncation dimension χ. The fitting function is $\lambda_\chi=\lambda_c+a\chi^{-b}$, where $\lambda_c=1.000\,15$, with $a=0.316\,12$ and $b=1.985\,65$. This indicates that we are able to locate the transition point accurately, with moderate computational cost. The accuracy may be further improved if the truncation dimension χ is increased.

$$H=\sum_{i=-\infty}^{\infty}(S_x^{[i]}S_x^{[i+1]}+\Delta_y S_y^{[i]}S_y^{[i+1]}+S_z^{[i]}S_z^{[i+1]}+hS_z^{[i]}), \quad (2)$$

where $S_\alpha^{[i]}$ $(\alpha=x,y,z)$ are the Pauli spin operators of the ith spin-$\frac{1}{2}$, Δ_y denotes the anisotropy in the internal spin space, and h is an external magnetic field. The model possesses a Z_2 symmetry, generated by the operation: $S_x^{[i]}\to -S_x^{[i]}$ and $S_y^{[i]}\to -S_y^{[i]}$. Note that $\Delta_y<1$ and $\Delta_y>1$ correspond to easy-plane and easy-axis behavior, respectively. The ordered phase in the easy-plane (easy-axis) case arises from an SSB along the $x(y)$ direction, with a nonzero order parameter, i.e., the magnetization $\langle S_x^{[i]}\rangle$ $(\langle S_y^{[i]}\rangle)$ below the critical field h_c. Here we shall choose $\Delta_y=0.25$, for which it is critical at $h=h_c$, with $h_c\sim 3.210(6)$ from the quantum Monte Carlo simulation [27].

V. SIMULATION RESULTS

In Fig. 1, we present the probability mass function for the quantum Ising model in a transverse magnetic field in the Z_2 symmetry-broken phase $(\lambda=1/2)$. Suppose a random variable K follows the binomial distribution with parameters n and p, then the probability of getting exactly k successes in n trials is given by the probability mass function: $\Pr(K=k)=C_n^k p^k(1-p)^{n-k}$, for $k=0,1,2,\ldots,n$, where $C_n^k=n!/[k!(n-k)!]$ is the binomial coefficient. Here, by a success we mean that the order parameter $\langle S_x^{[i]}\rangle$ is positive. Our data are presented for both $n=20$ and $n=40$, with the truncation dimension χ to be 8. This confirms that the probability for getting the ground state with the positive order parameter $\langle S_x^{[i]}\rangle$ each simulation run is $p=1/2$, as anticipated for the binomial distribution. Therefore, our results demonstrate that an SSB occurs in classical simulations of quantum systems on an infinite-size lattice in the context of the iMPS algorithm. This is in sharp contrast to algorithms that simulate finite-size lattice systems, which are forbidden to produce degenerate symmetry-breaking ground states, since an SSB *only* occurs in the infinite-size (thermodynamic) limit.

In Fig. 2 we plot the ground-state fidelity per lattice site, $d(\lambda_1,\lambda_2)$, for the quantum Ising model in a transverse field. Here, the transverse magnetic field strength λ is the control parameter. If we choose $\Psi(\lambda_2)$ as a reference state, with λ_2 in the Z_2 symmetry-broken phase (as shown here, $\lambda_2=0.9$), then $d(\lambda_1,\lambda_2)$ is able to distinguish two degenerate ground states, with a pseudo phase transition point λ_χ as a *bifurcation point* [28]. The critical value $\lambda_c=1.000\,15$ is determined from an extrapolation of the pseudo phase transition point λ_χ for the truncation dimension χ (see the inset in Fig. 2), which is quite close to the exact value 1. Therefore, the iMPS algorithm enables us to locate the transition point accurately from the computation of $d(\lambda_1,\lambda_2)$, with moderate computational cost. We stress that such a scaling for finite values of the truncation dimension χ has been discussed for the von Neumann entropy [29].

We have also presented $d(h_1,h_2)$ for the spin-$\frac{1}{2}$ XYX model in an external magnetic field on an infinite-size lattice in Fig. 3. Here, the external magnetic field h is the control parameter. If we choose $\Psi(h_2)$ as a reference state, with h_2 in the Z_2 symmetry-broken phase (as shown here, $h_2=3.2$), then $d(h_1,h_2)$ is able to distinguish two degenerate ground states, with a pseudo phase transition point h_χ as a *bifurcation point*. The critical point $h_c=3.204\,71$ is determined from an extrapolation of the pseudo phase transition point h_χ for the truncation dimension χ, as seen from the inset in Fig. 3.

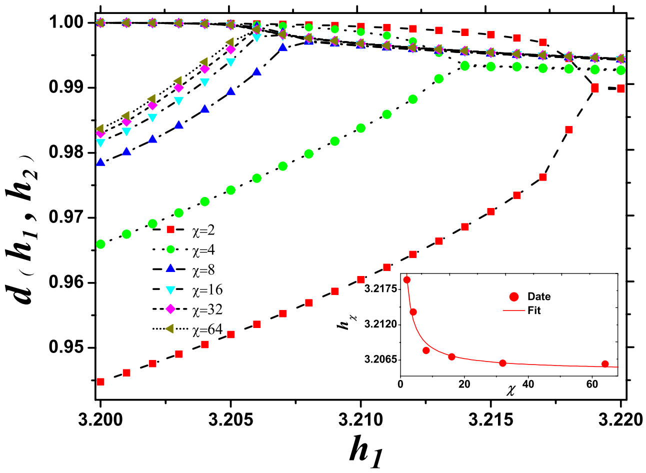

FIG. 3. (Color online) Main: the ground-state fidelity per lattice site, $d(h_1,h_2)$, as a function of the magnetic field strength h_1, with a fixed h_2 (h_2=3.2), for the spin-$\frac{1}{2}$ *XYX* model in an external magnetic field. Inset: the critical point h_c is determined from an extrapolation of the pseudo phase transition point h_χ for the truncation dimension χ. The fitting function is $h_\chi = h_c + a\chi^{-b}$, where h_c =3.204 71, with a=0.026 53 and b=0.860 03.

VI. SUMMARY

We have demonstrated that the iMPS algorithm may produce degenerate symmetry-breaking ground states arising from an SSB, each of which results from a randomly chosen initial state. It is shown that an SSB is reflected as a bifurcation in the ground-state fidelity per lattice site for quantum lattice systems undergoing QPTs with symmetry-breaking orders. Conceptually, this establishes the connection between the fidelity approach to QPTs and the singularity theory. Practically, it is also important since it makes possible to locate transition points without the need to compute the derivatives of the ground-state fidelity per lattice site with respect to the control parameter, which is usually a formidable task. We illustrated the general scheme in terms of the quantum Ising model in a transverse magnetic field and the spin-$\frac{1}{2}$ *XYX* model in an external magnetic field on an infinite-size lattice. However, it is applicable to any translationally invariant quantum lattice many-body systems in one spatial dimension.

Finally, it would be interesting to extend our investigation to quantum lattice systems in two and higher spatial dimensions, with the iMPS algorithm replaced by the iPEPS algorithm [18]. Given that the ground-state fidelity per lattice site may be computed in the context of the iPEPS algorithm [8], it is promising to carry the idea further to quantum lattice systems in two spatial dimensions. This is currently under active investigation [19].

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