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To cite this article: Yan-Wei Dai et al 2010 J. Phys. A: Math. Theor. 43 372001

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Ground-state fidelity and entanglement entropy for the quantum three-state Potts model in one spatial dimension

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Received 7 June 2010, in final form 13 July 2010
Published 4 August 2010
Online at stacks.iop.org/JPhysA/43/372001

Abstract

The ground-state fidelity per lattice site is computed for the quantum three-state Potts model in a transverse magnetic field on an infinite-size lattice in one spatial dimension in terms of the infinite matrix product state algorithm. It is found that, on the one hand, a pinch point is identified on the fidelity surface around the critical point, and on the other hand, the ground-state fidelity per lattice site exhibits bifurcations at pseudo critical points for different values of the truncation dimension, which in turn approach the critical point as the truncation dimension becomes large. This implies that the ground-state fidelity per lattice site enables us to capture spontaneous symmetry breaking when the control parameter crosses the critical value. In addition, a finite-entanglement scaling of the von Neumann entropy is performed with respect to the truncation dimension, resulting in a precise determination of the central charge at the critical point. Finally, we compute the transverse magnetization, from which the critical exponent $\beta$ is extracted from the numerical data.

PACS numbers: 03.67.-a, 03.65.Ud, 03.67.Hk

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The classical two-dimensional statistical lattice $q$-state Potts model [1, 2] was introduced as a generalization of the celebrated Ising model. In 1973, Baxter [3] computed the free energy of the Potts model at the critical temperature, and showed that it undergoes a continuous phase transition for $q \leq 4$, and a first-order phase transition for $q > 4$. In the context of the transfer matrix method [4], the model may be rephrased as a one-dimensional quantum lattice system with its Hamiltonian describing the interaction between spins in a transverse magnetic field. It is known that the quantum version of the model exhibits a continuous quantum phase transition.
(QPT) for $q \leq 4$ and a first-order QPT for $q > 4$, due to the emergence of long-range order arising from symmetry spontaneous breaking (SSB) associated with the symmetry group $Z_q$.

In the symmetry-broken phase, the model is characterized by the nonzero values of a local order parameter.

Recently, a new perspective from quantum information science emerges for investigating QPTs in a variety of quantum many-body lattice systems, namely the fidelity approach to QPTs [5–9]. As argued in [6–8], the ground-state fidelity per site is able to capture drastic changes of the ground-state wavefunctions around a critical point, with a pinch point as its signature. In addition, it was shown [10] that, for a QPT arising from an SSB, a bifurcation occurs in the ground-state fidelity per site, with a pinch point identified as a bifurcation point. In fact, the ground-state fidelity per site is able to describe QPTs arising from an SSB [10], the Kosterlitz–Thouless transition [11] and topological QPTs in the Kitaev model [12]. The advantage of the ground-state fidelity per site over local order parameters lies in the fact that the ground-state fidelity per site is universal in the sense that it is not model-dependent, in contrast to model-dependent order parameters characterizing QPTs in the context of the conventional Ginzburg–Landau–Wilson paradigm. However, for systems with SSB order, only discrete $Z_2$ symmetry has been specifically addressed. Therefore, it is desirable to investigate quantum many-body lattice systems which undergo QPTs with other symmetry groups.

In this communication, we investigate the quantum three-state Potts model in a transverse magnetic field in one spatial dimension. First, we demonstrate that the infinite matrix product state (iMPS) algorithm [13] on infinite-size lattices produces three 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, on the one hand, there is a pinch point on the fidelity surface around the critical point, and on the other hand, the ground-state fidelity per lattice site exhibits bifurcations at pseudo critical points for different values of the truncation dimension, which in turn approach the critical point as the truncation dimension becomes large. This confirms that for the quantum three-state Potts model in a transverse magnetic field in one spatial dimension, the ground-state fidelity per lattice site enables us to capture SSB when the control parameter crosses the critical value. Therefore, for quantum lattice systems undergoing QPTs with the symmetry group $Z_3$, an SSB is reflected as a bifurcation in the ground-state fidelity per lattice site [14]. In addition, a finite-entanglement scaling [15, 16] of the von Neumann entropy is performed with respect to the truncation dimension, resulting in a precise determination of the central charge at the critical point. Finally, we compute the transverse magnetization, from which the critical exponent is extracted from the numerical data.

2. Model

We consider the three-state quantum Potts model in a transverse magnetic field on an infinite-size lattice in one spatial dimension [4]. It is described by the Hamiltonian

$$H = -\sum_{i=-\infty}^{\infty} \left( \sum_{\alpha=1,2} M^{[i]}_{\alpha,\alpha} M^{[i+1]}_{\alpha,\alpha} + \lambda M^{[i]}_{z} \right),$$

(1)

where $\lambda$ is the transverse magnetic field and $M^{[i]}_{\alpha} (\alpha = x, z)$ are the Potts spin matrices:

$$M_z = \begin{pmatrix} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad M_{x,1} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$
and

\[ M_{x,2} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}. \]

The model is invariant with respect to the operations \( M_{x,1} \rightarrow \omega M_{x,1} \), \( M_{x,2} \rightarrow \omega^2 M_{x,2} \) and \( M_Z \rightarrow M_Z \), where \( \omega = \exp(i2\pi/3) \), for all the sites simultaneously. Therefore, it possesses the \( Z_3 \) symmetry. As is well known, it undergoes a QPT, with a critical point at \( \lambda_c = 1 \).

3. Infinite matrix product state algorithm and spontaneous symmetry breaking

For completeness, let us briefly recall the key ingredients of the variational MPS algorithm initiated by Vidal [13] to compute the ground-state wavefunctions for quantum many-body systems on an infinite-size lattice in one spatial dimension, which itself is an infinite-size variant of the MPS algorithm [17, 18] on a finite-size lattice in one spatial dimension. Assume that the Hamiltonian is translationally invariant, and consists of the nearest-neighbor interactions: \( H = \sum_i h[i,i+1] \), with \( h[i,i+1] \) being the nearest-neighbor two-body Hamiltonian density. Attached to each site is a three-index tensor \( \Gamma^s_{A\ell r} \) and to each bond a diagonal (singular value) matrix \( \lambda_{A,\ell} \), depending on the evenness and oddness of the \( i \)th 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 \( \ell, r = 1, \ldots, \chi \), with \( \chi \) being the truncation dimension.

The issue to generate the ground-state wavefunction for a given Hamiltonian \( H \) amounts to computing the imaginary time evolution \( |\Psi(\tau)\rangle = \exp(-H\tau)|\Psi(0)\rangle/|\exp(-H\tau)|\Psi(0)\rangle| \). For large enough \( \tau \) and a generic initial state \( |\Psi(0)\rangle \), it yields a good approximation to the ground-state wavefunction, as long as there is a gap in the spectrum of the system. Exploiting the Suzuki–Trotter decomposition [19], one may reduce the imaginary time evolution operator to a product of two-site evolution operators that only act on the sites \( i \) and \( i + 1 \): \( U(i,i+1) = \exp(-h[i,i+1]\Delta\tau), \Delta\tau \ll 1 \). Note that, after absorbing a two-site gate \( U(i,i+1) \), the state is no longer in the MPS representation and it also breaks the translational invariance under one-site shifts. In order to recover the MPS representation, it is necessary to perform a singular value decomposition of a matrix contracted from one \( \Gamma^s_{A\ell r} \), one \( \Gamma^s_{B\ell r} \), one \( \lambda_A \) and two \( \lambda_B \)'s, and only the \( \chi \) largest singular values are retained. This yields the new tensors \( \Gamma^s_{A\ell r}, \Gamma^s_{B\ell r} \) and \( \lambda_A \), 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 yields the system’s ground-state wavefunction in the MPS representations.

As argued in [10], for a quantum many-body lattice 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, in the sense that the state is generated by filling the MPS matrices with random numbers.

For the three-state quantum Potts model in a transverse magnetic field on an infinite-size lattice in one spatial dimension, we may restrict ourselves to consider the discrete symmetry group \( Z_3 \). In the \( Z_3 \) symmetric phase, the ground state is nondegenerate, whereas in the \( Z_3 \) symmetry-broken phase, three degenerate ground states arise from classical simulations of the model in the context of the iMPS algorithm.
In figure 1, we present the probability mass function for the quantum Potts model in a transverse magnetic field in the $Z_3$ symmetry-broken phase ($\lambda = 1/3$). The probability mass function is defined as the probability of getting exactly $k$ successes in $n$ trials: $\Pr(K = k) = C_n^k p^k (1 - p)^{n-k}$, 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 $\langle M_{x,1}^i + M_{x,2}^i \rangle/2$ is a positive number. Our data are presented, in the cases of both $n = 30$ and $n = 60$, for the quantum Potts model in a transverse magnetic field in the $Z_3$ symmetry-broken phase ($\lambda = 1/3$). Here, the truncation dimension is $\chi = 4$. This confirms that the probability of getting the ground-state wavefunction with a positive $\langle M_{x,1}^i + M_{x,2}^i \rangle/2$ order parameter is $p = 1/3$. Therefore, a $Z_3$ SSB occurs in classical simulations of the quantum Potts model in a transverse magnetic field in the $Z_3$ symmetry-broken phase in the context of the iMPS algorithm.
which is seen to be well defined in the thermodynamic limit even if $F(\lambda_1, \lambda_2)$ trivially becomes zero. It 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 $0 \leq d(\lambda_1, \lambda_2) \leq 1$.

In figure 2, we plot the ground-state fidelity per site, $d(\lambda_1, \lambda_2)$, for the quantum three-state Potts model in a transverse field as a function of $\lambda_1$ and $\lambda_2$. Here, a pinch point, as expected, is seen in the ground-state fidelity surface around the exact critical point $\lambda_c = 1$. Note that a pinch point was first introduced in [6, 8] as an intersection of two singular lines to characterize phase transition points. Our result furnishes another example for the connection between pinch points on a fidelity surface and critical points for a quantum many-body lattice system undergoing a QPT [6].

5. Bifurcation in the ground-state fidelity per lattice site

As argued in [10], a bifurcation occurs for the ground-state fidelity per lattice site, $d(\lambda_1, \lambda_2)$. More precisely, if we choose $\Psi(\lambda_2)$ as a reference state, with $\lambda_2$ in the $Z_3$ symmetric phase, then the ground-state fidelity per lattice site, $d(\lambda_1, \lambda_2)$, cannot distinguish three degenerate ground states in the $Z_3$ symmetry-broken phase. However, if we choose $\Psi(\lambda_2)$ as a reference state, with $\lambda_2$ in the $Z_3$ symmetry-broken phase, then the ground-state fidelity per lattice site, $d(\lambda_1, \lambda_2)$, can be used to distinguish three degenerate ground states. Therefore, for a given truncation dimension $\chi$, a pseudo phase transition point $\lambda_\chi$ manifests itself as a bifurcation point [14]. An extrapolation to $\chi = \infty$ determines the critical point $\lambda_c$. That is, the pinch point is identified as a bifurcation point.

In figure 3, we plot the ground-state fidelity per lattice site, $d(\lambda_1, \lambda_2)$, for the quantum Potts model in a transverse magnetic field. Here, the transverse magnetic field strength $\lambda$ is the control parameter. If we choose $\Psi(\lambda_2)$ as a reference state, with $\lambda_2$ in the $Z_3$ symmetry-broken phase, then $d(\lambda_1, \lambda_2)$ is able to distinguish three degenerate ground states, with a pseudo phase transition point $\lambda_\chi$ as a bifurcation point [10]. We have chosen $\lambda_2 = 0.9$ as a specific example. The critical value $\lambda_\chi = 1.00015$ is determined from an extrapolation of the pseudo phase transition point $\lambda_\chi$ for the truncation dimension $\chi$ (see the inset in figure 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 the ground-state fidelity per site, $d(\lambda_1, \lambda_2)$, with moderate computational cost.
An intriguing feature of the bifurcation points for the ground-state fidelity per lattice site, $d(\lambda_1, \lambda_2)$, as seen in figure 3, is that $d(\lambda_1, \lambda_2)$ between different symmetry breaking ground states in the same phase is always lower than that between two ground states from different phases. However, this is not unexpected. Physically, this simply means that two degenerate symmetry breaking ground states in the same symmetry-broken phase are more distinguishable than two ground states from different phases.

6. von Neumann entropy

The von Neumann entropy is a measure of a bipartite entanglement present in a quantum state, whose behavior is, in many occasions, universal [20]. The von Neumann entropy of a pure state for a system partitioned into two parts $A$ and $B$ is defined as $S = -\text{Tr} \rho_A \log \rho_A = -\text{Tr} \rho_B \log \rho_B$, where $\rho_A$ ($\rho_B$) is the reduced density matrix of the subsystem $A$($B$). In the iMPS representation, the von Neumann entropy for a semi-infinite interval becomes

$$S = -\text{Tr} \lambda^2 \log \lambda^2. \quad (3)$$

Here, $\lambda$ is a diagonal (singular value) matrix. As discussed in [15, 16], at criticality, there is a simple scaling relation between the von Neumann entropy $S$ and the truncation dimension $\chi$:

$$S \sim \frac{c \kappa}{6} \log \chi, \quad (4)$$

where $c$ is the central charge and $\kappa$ is the so-called finite-entanglement scaling exponent, which roughly takes the value $[16]$:

$$\kappa \approx \frac{6}{c\left(\sqrt{\frac{12}{c} + 1}\right)}. \quad (5)$$
In figure 4, we plot the correlation length, $\xi$, as a function of the truncation dimension $\chi$ for the three-state Potts model at the critical point $\lambda = 1$. In passing, we point out that the correlation length, $\xi$, is extracted according to a scheme advocated in [15]. The value of the exponent $\kappa$ is extracted from our data, where the fitting function is $a\chi^{\kappa}$ with $a$ and $\kappa$ being left as the free parameters. We have $\kappa = 1.47(1)$ and $a = 0.21(3)$. The exponent $\kappa$ thus obtained is reasonably well compared with $\kappa = 1.553(0)$ predicted from equation (5).

In figure 5, the von Neumann entropy is plotted for the quantum three-state Potts model in one spatial dimension. As expected, it diverges with the truncation dimension $\chi$ logarithmically. That is, for a given $\chi$, $S$ scales as $\log \chi$. Our numerical results for the entropy $S_\chi$ at $\lambda = 1$ as a function of $\chi$ accurately fit into the scaling law (4), with $c \approx 0.789(9)$, which is quite close to the exact value $c = 4/5$. 
7. Magnetization

The iMPS algorithm makes it possible to extract an (optimized) local order parameter, according to a general scheme advocated in [21]. In fact, once the critical field \( \lambda_c \) is determined, one may choose two representative ground states: one for an external transverse magnetic field \( \lambda \) less than the critical field \( \lambda_c \) and the other for an external transverse magnetic field \( \lambda \) greater than the critical field \( \lambda_c \). Then one computes the single-site reduced density matrix \( \rho_1 \) for the model on an infinite-size lattice for two different values of the external transverse magnetic field \( \lambda \), corresponding to \( \lambda > \lambda_c \) and \( \lambda < \lambda_c \), respectively. It turns out that the one-site reduced density matrix \( \rho_1 \) displays different nonzero-entry structures in two phases, with \( \langle M_{x,1} + M_{x,2} \rangle/2 \) being zero for \( \lambda > \lambda_c \) and nonzero for \( \lambda < \lambda_c \).

In figure 6, the spontaneous magnetization, which itself is the local order parameter, is computed for the quantum three-state Potts model in one spatial dimension. From this we see that the pseudo critical points are getting closer to the exact critical point \( \lambda_c = 1 \) with increasing \( \chi \). A fit for the critical exponent of the model gives \( \beta = 0.1167 \). The value is within less than 6% compared to the exact value \( \beta = 1/9 \) of the critical exponent for the Potts model.

8. Conclusions

We have investigated the ground-state fidelity for the quantum three-state Potts model in a transverse magnetic field in one spatial dimension in the context of the iMPS algorithm. The iMPS algorithm produces three degenerate symmetry-breaking ground states arising from an SSB, each of which results from a randomly chosen initial state. As such, we have shown that, on the one hand, a pinch point is identified on the fidelity surface around the critical point, and on the other hand, the ground-state fidelity per lattice site exhibits bifurcations at pseudo critical points for different truncation dimensions, which in turn approach the critical point as the truncation dimension gets large. In addition, a finite-entanglement scaling of the von
Neumann entropy has been performed with respect to the truncation dimension, resulting in a precise determination of the central charge at the critical point. Finally, we computed the transverse magnetization to extract the critical exponent $\beta = 0.1167$ from the numerical data.

Acknowledgments

This work is supported in part by the National Natural Science Foundation of China (grant nos 10774197 and 10874252), the Natural Science Foundation of Chongqing (grant no CSTC2008BC2023), and Chongqing University Postgraduates Science and Innovation Fund (project no 200911C1A0140330).

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