Kosterlitz–Thouless phase transition and ground state fidelity: a novel perspective from matrix product states

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Abstract. The Kosterlitz–Thouless transition is studied from the representation of the system’s ground state wavefunctions in terms of matrix product states for a quantum system on an infinite-size lattice in one spatial dimension. It is found that, in the critical regime for a one-dimensional quantum lattice system with continuous symmetry, the newly developed infinite matrix product state algorithm automatically leads to infinite degenerate ground states, due to the finiteness of the truncation dimension. This results in pseudo continuous symmetry spontaneous breakdown, which allows the introduction of a pseudo-order parameter that must be scaled down to zero, in order to be consistent with the Mermin–Wegner theorem. We also show that the ground state fidelity per lattice site exhibits a catastrophe point, thus resolving a controversy regarding whether or not the ground state fidelity is able to detect the Kosterlitz–Thouless transition.

Keywords: quantum phase transitions (theory)
1. Introduction

The Kosterlitz–Thouless (KT) transition [1], an infinite order transition from a critical phase to a gapful phase, is ubiquitous in quantum systems on infinite-size lattices in one spatial dimension. It describes one of the instabilities of the Luttinger liquid induced by a marginal perturbation. Remarkably, it does not arise from the long-range ordering, thus it falls outside of the conventional Landau–Ginzburg–Wilson paradigm, in which the most fundamental notion is spontaneous symmetry breaking (SSB) [2,3], with the symmetry-broken phase characterized by a nonzero local order parameter. Indeed, the type of internal order that a system possesses is profoundly affected by its dimensionality. In quantum field theory, the Mermin–Wegner theorem states that continuous symmetries cannot be spontaneously broken in systems with local interactions in one spatial dimension [4]. That is, in quantum systems with a continuous symmetry in one spatial dimension, a genuine long-range order is destroyed by quantum fluctuations. Instead, a quasi-long-range order occurs in the critical phase, which is characterized by a power-law decay in correlation functions.

The peculiarity of the KT transition makes it very difficult to map out the ground state phase diagrams for various quantum lattice systems in one spatial dimension. Indeed, a numerical analysis of the KT transition suffers from pathological problems. One of these problems is that the finite-size scaling technique [5], which is successful for second order quantum phase transitions (QPTs) [6,7], cannot be applied to the KT transition [8], since there are logarithmic corrections from the marginal perturbation. This motivated Nomura and Okamoto [9] to develop the so-called level spectroscopy to overcome these difficulties.
by combining the renormalization group, conformal field theory and the symmetry. This raises an intriguing question as to whether or not there is a unifying practical approach to different types of QPTs.

In this letter, we address this issue from a novel perspective. The new inputs come from recent advances in both classical simulations of quantum lattice systems and our understanding of QPTs. First, a tensor network (TN) representation of quantum many-body wavefunctions provides an efficient way to classically simulate quantum many-body systems, which include matrix product states (MPSs) in one spatial dimension and projected entangled-pair states (PEPSs) in two or more spatial dimensions. Second, two novel approaches to study QPTs have been proposed in terms of both entanglement [10] and fidelity [11]–[16]. In [12,13], it was argued that the ground state fidelity per lattice site, in combination with a practical way to compute it using the TN algorithms for translationally invariant infinite-size systems, is able to capture the many-body physics underlying various quantum lattice systems in condensed matter.

Although an MPS is well suited for the description of a gapped quantum state, it remains mysterious how it works for quantum states in the gapless regime. This casts doubts on the applicability of the TN algorithms to the study of the KT transition. Our approach is based on the observation that, in the gapless regime, the newly developed infinite MPS (iMPS) algorithm automatically leads to infinite degenerate ground states, due to the finiteness of the truncation dimension. This results in pseudo continuous SSB\(^1\), which allows the introduction of a pseudo-order parameter that must be scaled down to zero, in order to be consistent with the Mermin–Wegner theorem. We also show that the ground state fidelity per lattice site exhibits a catastrophe point\(^2\) at a pseudo critical point for any finite truncation dimension. Normally, an extrapolation to infinite truncation dimension should be performed to determine the KT transition point. This resolves a controversy regarding whether or not the ground state fidelity is able to detect the KT transition [15,16].

\section{Matrix product states on an infinite-size lattice in one spatial dimension and continuous symmetries}

The iMPS algorithm is a variational algorithm to compute the MPS representations of ground state wavefunctions for translationally invariant quantum systems on an infinite-size lattice in one spatial dimension [18]. Assume that the Hamiltonian takes the form \(H = \sum_i h[i,i+1]\), with \(h[i,i+1]\) being the nearest-neighbor two-body Hamiltonian density. The problem of finding the system’s ground state wavefunctions amounts to computing the imaginary time evolution for a given initial state \(|\Psi(0)\rangle\): \(|\Psi(\tau)\rangle = \exp(-H\tau)|\Psi(0)\rangle/|\exp(-H\tau)|\Psi(0)\rangle\). An efficient way to do this is based on the observation that the imaginary time evolution operator is reduced to a product of two-site evolution operators acting on sites \(i\) and \(i+1\): \(U(i,i+1) = \exp(-h[i,i+1]\delta\tau), \delta\tau \ll 1\), as follows from the Suzuki–Trotter decomposition [19], and the fact that any wavefunction admits an MPS representation in a canonical form: attached to each site is a three-

\(^1\) The term ‘pseudo SSB’ describes a numerical phenomenon, in which an SSB is induced by the truncation in the iMPS algorithm. It vanishes when the truncation is removed.

\(^2\) Catastrophe theory studies and classifies phenomena characterized by sudden changes in behavior arising from small variations in control parameters. For a review, see [17].
index tensor $\Gamma^s_{Alr}$ or $\Gamma^s_{Blr}$, and to each bond a diagonal matrix $\lambda_A$ or $\lambda_B$, 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 $l$ and $r$ denote the bond indices, $l, r = 1, \ldots, \chi$, with $\chi$ being the truncation dimension. The effect of a two-site gate $U(i, i + 1)$ may be absorbed by performing a singular value decomposition. This allows the tensors involved in the MPS representation to be updated. Repeating this procedure until the ground state energy converges, one may generate the system’s ground state wavefunctions in the MPS representation.

It is known that the iMPS algorithm yields the best approximation to the ground state wavefunction (for a fixed truncation dimension $\chi$), as long as the ground state is gapful. However, it is surprising to see that it also works for quantum lattice systems with continuous symmetries in a gapless regime. The key point here is that continuous symmetries and translational invariance under one-site shifts cannot be maintained simultaneously during the imaginary time evolution\(^3\). Indeed, in order to mimic the gaplessness of excitations in the gapless regime, the iMPS algorithm resorts to the Goldstone mode. That is, the best approximation to the ground state wavefunction is not unique, if the translational invariance under one-site shifts is maintained\(^4\). Instead, infinite degenerate ground states are generated, each of which breaks the continuous symmetry. From now on, we restrict ourselves to the symmetry group $U(1)$.

3. **Pseudo continuous symmetry spontaneous breakdown and pseudo-order parameters**

For a $U(1)$ invariant quantum system on an infinite-size lattice in one spatial dimension the iMPS algorithm automatically produces infinite degenerate ground states, each of which breaks the $U(1)$ symmetry. Moreover, the symmetry breakdown results from the fact that an initial state has been chosen randomly. That is, a phenomenon occurs which shares all the features of an SSB [2,3]. Indeed, the implication of an SSB is two-fold: 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. In addition, such a ‘symmetry-breaking order’ may be quantified by introducing a local ‘order parameter’, which may be read off from the reduced density matrix on a local area [21]. However, this is in apparent contradiction with the Mermin–Wegner theorem, which states that continuous symmetries cannot be spontaneously broken for quantum systems in one spatial dimension [4]. To resolve this contradiction, one has to require that the ‘order parameter’ must be scaled down to zero when the truncation dimension $\chi$ tends to $\infty$. In order to distinguish them from a genuine SSB and a local order parameter, we introduce the notions of a *pseudo* SSB and a pseudo-order parameter. In this scenario, the Goldstone mode survives as gapless excitations in the critical phase when the truncation dimension goes to $\infty$. Thus, the Luttinger liquid may be characterized as a limiting case of the conventional symmetry-breaking order. That is, the long-range order vanishes when the truncation dimension becomes $\infty$.

\(^3\) For an antiferromagnetic spin system, the translational invariance under one-site shifts should be accompanied by spin reversal at all the sites simultaneously.

\(^4\) There is another choice that maintains continuous symmetries, but breaks the translational invariance under one-site shifts. See [20].
4. Ground state fidelity per lattice site

Suppose that a $U(1)$ invariant quantum lattice system undergoes the KT transition when a control parameter $\lambda$ crosses a critical point $\lambda_c$. Let us see whether or not the ground state fidelity per lattice site is able to detect it. The ground state fidelity per lattice site, $d(\lambda_1, \lambda_2)$, is defined as 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 \cite{12,13}. 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 $L$ the number of sites in a finite-size lattice. Remarkably, $d(\lambda_1, \lambda_2)$ 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 $0 \leq d(\lambda_1, \lambda_2) \leq 1$.

In the $U(1)$ symmetric phase, the ground state is non-degenerate\(^5\), whereas in the $U(1)$ symmetry-broken phase, infinite degenerate ground states arise. This implies that, if we choose $\Psi(\lambda_2)$ as a reference state, with $\lambda_2$ in the $U(1)$ symmetric phase, then the ground state fidelity per lattice site, $d(\lambda_1, \lambda_2)$, cannot distinguish infinite degenerate ground states in the $U(1)$ symmetry-broken phase. This follows from the fact that $\langle \Psi(\lambda_2) | \Psi_\eta(\lambda_1) \rangle = \langle \Psi_\eta(\lambda_2) | U(\xi) | \Psi_\eta(\lambda_1) \rangle = \langle \Psi(\lambda_2) | \Psi_\eta(\lambda_1 + \xi) \rangle$, with $U(\xi)$ being an element of the symmetry group $U(1)$, and the subscript $\eta$ in $|\Psi_\eta(\lambda)\rangle$ labeling the eigenstates of the $U(1)$ generator. However, if we choose $\Psi(\lambda_2)$ as a reference state, with $\lambda_2$ in the $U(1)$ symmetry-broken phase, then $d(\lambda_1, \lambda_2)$ is able to distinguish infinite degenerate ground states. Therefore, the phase transition point $\lambda_c$ manifests itself as a catastrophe point for any finite $\chi$. The catastrophe point disappears as $\chi$ tends to $\infty$. However, the critical point $\lambda_c$ may be determined by performing a scaling analysis with reasonably small $\chi$\(^6\).

5. Examples

The first example we shall investigate is the spin $1/2$ XXZ model described by the Hamiltonian

$$H = \sum_{i=-\infty}^{\infty} \left( S_x^{[i]} S_x^{[i+1]} + S_y^{[i]} S_y^{[i+1]} + \Delta S_z^{[i]} S_z^{[i+1]} \right),$$

where $S_\alpha^{[i]}$ ($\alpha = x, y, z$) are the Pauli spin operators at the site $i$, and $\Delta$ denotes the anisotropy in the internal spin space. The model is in the critical regime (CR) for

\(^5\) We emphasize that there are two different types of KT transition: normal and generic. In the normal KT transition, there is no SSB in the gapful phase (see the spin 1 XXZD model in section 5). But the generic KT transition is accompanied by an SSB of the discrete symmetry group $Z_N$ in the gapful phase (see the spin 1/2 XXZ model in section 5). Here, we focus on the normal KT transition. However, the only difference for the generic KT transition is that in the $U(1)$ symmetric phase, degenerate ground states arise due to the SSB of $Z_N$. Following \cite{25}, if we choose $\Psi(\lambda_2)$ as a reference state, with $\lambda_2$ in the $Z_N$ symmetry-broken phase, then $d(\lambda_1, \lambda_2)$ is able to distinguish those degenerate ground states.

\(^6\) It is possible to locate the critical point from the von Neumann entropy, a bipartite entanglement measure. However, the von Neumann entropy is fully determined by the singular value matrices $\lambda_A$ and $\lambda_B$, which are the same due to the fact that the translational invariance under one-site shifts is maintained. Because all the information concerning a pseudo SSB is encoded in $\Gamma_{\Lambda_{1\tau}}$ and $\Gamma_{\Lambda_{B\tau}}$, the von Neumann entropy fails to detect a pseudo SSB.
**Table 1.** The one-site reduced density matrices for the spin 1/2 XXZ model ($\Delta = 0$) and the spin 1 XXZD model with uniaxial single-ion anisotropy ($J_z = -0.5, D = -0.3$): $\rho^{[i]}_{\text{XXZ}} = \frac{1}{2} I + \alpha S_x^{[i]} + \beta S_z^{[i]} + \gamma S_y^{[i]}$ and $\rho^{[i]}_{\text{XXZD}} = \frac{1}{3}(1-2\beta)I + \alpha S_x^{[i]} + \beta(S_z^{[i]})^2 + \sqrt{2}\gamma S_x^{[i]} + \sqrt{2}\delta S_y^{[i]} + \mu((S_x^{[i]})^2 - (S_y^{[i]})^2) + \nu(S_z^{[i]}S_y^{[i]} + S_y^{[i]}S_z^{[i]}).

The two degenerate ground states originating from two randomly chosen initial states are connected via $S_x^{[i]} = \cos \theta S_x^{[i]} + \sin \theta S_y^{[i]}, S_y^{[i]} = -\sin \theta S_x^{[i]} + \cos \theta S_y^{[i]}$, with $\theta = 77.140$ for the spin 1/2 XXZ model and $\theta = 72.001$ for the spin 1 XXZD model.

| Model   | $\alpha$ | $\beta$ | $\gamma$ | $\delta$ | $\mu$ | $\nu$ |
|---------|----------|---------|----------|----------|-------|-------|
| XXZ     | 0        | -0.00186| 0.17359  | —        | —     | —     |
| Spin 1/2| 0.16882  | 0.04045 | —        | —        | —     | —     |
| XXZD    | -0.24659 | -0.27287| 0.00314  | 0.08843  | -0.00204| —     |
| Spin 1  | -0.24659 | -0.08133| 0.26049  | -0.07274 | -0.05033| —     |

$\Delta \in (-1, 1]$, with the same universality class as a free bosonic field theory, and exhibits antiferromagnetic (AF) and ferromagnetic (FM) orders, respectively, for $\Delta > 1$ and $\Delta < -1$. Besides a continuous $U(1)$ symmetry, the model also enjoys a $Z_2$ symmetry, generated by the operation $S_x^{[i]} \leftrightarrow S_y^{[i]}$ and $S_z^{[i]} \rightarrow -S_z^{[i]}$.

The second example is the spin 1 XXZD model with uniaxial single-ion anisotropy:

$$H = \sum_{i=-\infty}^{\infty} \left( S_x^{[i]}S_x^{[i+1]} + S_y^{[i]}S_y^{[i+1]} + J_zS_z^{[i]}S_z^{[i+1]} \right) + D \sum_{i=-\infty}^{\infty} (S_z^{[i]}S_z^{[i]})^2, \quad (2)$$

where $S_x^{[i]}$ ($\alpha = x, y, z$) are the spin 1 operators at the lattice site $i$, and $J_z$ and $D$ are the Ising-like and single-ion anisotropies, respectively. For $J_z = -1/2$, there are two phase transitions, i.e., the KT transition from the large-$D$ (LD) to a CR at $D \sim 0.693$, and a first order QPT from the CR to an FM phase at $D \sim -1.184$, as $D$ varies from $\infty$ to $-\infty$ [22].

**6. Simulation results**

In table 1, we present the specific coefficients in the one-site reduced density matrices for the spin 1/2 XXZ model ($\Delta = 0$) and the spin 1 XXZD model with uniaxial single-ion anisotropy ($J_z = -0.5, D = -0.3$): $\rho^{[i]}_{\text{XXZ}} = \frac{1}{2} I + \alpha S_x^{[i]} + \beta S_z^{[i]} + \gamma S_y^{[i]}$ and $\rho^{[i]}_{\text{XXZD}} = \frac{1}{3}(1-2\beta)I + \alpha S_x^{[i]} + \beta(S_z^{[i]})^2 + \sqrt{2}\gamma S_x^{[i]} + \sqrt{2}\delta S_y^{[i]} + \mu((S_x^{[i]})^2 - (S_y^{[i]})^2) + \nu(S_z^{[i]}S_y^{[i]} + S_y^{[i]}S_z^{[i]}).

The two degenerate ground states originating from two randomly chosen initial states are connected via $S_x^{[i]} = \cos \theta S_x^{[i]} + \sin \theta S_y^{[i]}, S_y^{[i]} = -\sin \theta S_x^{[i]} + \cos \theta S_y^{[i]}$, with $\theta = 77.140$ for the spin 1/2 XXZ model (the fidelity per lattice site between them is 0.9976) and $\theta = 72.001$ for the spin 1 XXZD model (the fidelity per lattice site between them is 0.9925). The iMPS simulations are performed for a randomly chosen initial state, with $\chi$ set to be 16.

We may choose $\langle \langle S_x^{[i]} \rangle, \langle S_y^{[i]} \rangle \rangle$ as the pseudo-order parameter for both the models\footnote{Another choice of the pseudo-order parameter for the spin 1 XXZD model is $\langle (S_x^{[i]})^2 \rangle, \langle S_x^{[i]}S_y^{[i]} + S_y^{[i]}S_z^{[i]} \rangle$.}

In figures 1(a) and (b), we plot the magnitude $O_\chi = \sqrt{\langle S_x^{[i]} \rangle^2 + \langle S_y^{[i]} \rangle^2}$ of the pseudo-order parameter.
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Figure 1. Main figure: (a) the magnitude $O_\chi$ of the pseudo-order parameter $(\langle S_x^{[i]} \rangle, \langle S_y^{[i]} \rangle)$ for the spin 1/2 XXZ model and (b) that for the spin 1 XXZD model (with a fixed $J_z = -1/2$). The iMPS simulations are performed for a randomly chosen initial state, with the truncation dimension $\chi$ to be 8, 16, 32, and 50. Note that the pseudo-order parameter is discontinuous even at $\Delta = 1$ for the XXZ model. However, this is an artifact of the iMPS algorithm. Inset: the pseudo-order parameter is scaled down to zero, according to $O_\chi = a\chi^{-b(1+c\chi^{-1})}$, in the critical phase, in the right-top inset in (a) for the XXZ model (with $a = 0.7744, 0.8565, 0.9363, b = 0.3265, 0.2280, 0.1267, c = 0.4216, 0.3872, 0.1780$ for $\Delta = 0.4, -0.4, -0.8$, respectively), and the middle-bottom inset in (b) for the XXZD model (with $a = 0.9308, 0.9942, 0.9814, b = 0.1180, 0.0858, 0.0607, c = 0.1505, 0.0015, 0.0608$ for $D = 0.4, -0.4, -0.8$, respectively). Moreover, an extrapolation to $\chi = \infty$ is performed for the pseudo transition points (at which the pseudo-order parameter becomes zero), yielding the KT transition point $(D = 0.827)$ for the XXZD model in the right-top inset in (b).

Parameter for the spin 1/2 XXZ model and the spin 1 XXZD model (with a fixed $J_z = -1/2$), respectively. The iMPS simulations are performed for a randomly chosen initial state, with the truncation dimension $\chi$ to be 8, 16, 32, and 50. Note that the pseudo-order parameter is discontinuous even at $\Delta = 1$ for the XXZ model. However, this is an artifact of the iMPS algorithm. In fact, the pseudo-order parameter must be

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scaled down to zero, to keep consistency with the Mermin–Wegner theorem. Therefore, we require \( O_\chi = ax^{-b}(1 + c\chi^{-d}) \) to be valid. In the critical phase, such a fitting yields \( a = 0.7744, 0.8565, 0.9363, b = 0.3265, 0.2280, 0.1267, c = 0.4216, 0.3872, 0.1780 \) for the XXZ model with \( \Delta = 0.4, -0.4, -0.8 \), respectively (as shown in the right-top inset in (a)), and \( a = 0.9308, 0.9942, 0.9814, b = 0.1180, 0.0858, 0.0607, c = 0.1505, 0.0015, 0.0608 \) for the XXZD model with \( D = 0.4, -0.4, -0.8 \), respectively (as shown in the middle-bottom inset in (b)).

We have also performed an extrapolation to \( \chi = \infty \) for the pseudo transition points (at which the pseudo-order parameter becomes zero), yielding the transition point \( D = 0.827 \) for the XXZD model (see the right-top inset in figure 1(b)), besides two transitions at \( \Delta = -1 \) and \( \Delta = 1 \), respectively, for the spin 1/2 XXZ model, and the other transition point at \( D = -1.184 \) for the spin 1 XXZD model. Note that the transition points are determined quite precisely, compared to the known exact results for the XXZ model. For the XXZD model, the transition point \( D = -1.184 \) is precise, compared to the previous result [22], but the transition point \( D = 0.827 \) turns out to be larger than \( D \sim 0.693 \) from the level spectroscopy [22].

Here, we stress that the pseudo-order parameter alone is not sufficient to determine the universality class of each transition. However, its occurrence is a *defining* character of a critical regime, i.e., the Luttinger liquid phase. Actually, one may determine the central charge \( c = 1 \) by performing a finite-entanglement scaling analysis of the von Neumann entropy. As already mentioned, the Goldstone mode, arising from a continuous \( U(1) \) SSB, survives as gapless excitations in the critical phase when the truncation dimension goes to \( \infty \). In order to distinguish the first order transitions from continuous transitions including the KT transition, we turn to the computation of the ground state fidelity per lattice site. Actually, as shown in [12, 13], the ground state fidelity per lattice site is discontinuous for first order QPTs.

Our simulation results for the ground state fidelity per lattice site demonstrate that the transition points \( \Delta = -1 \) for the XXZ model and \( D = -1.184 \) for the XXZD model are discontinuous. Here, we focus on the transition points \( \Delta = 1 \) for the XXZ model and \( D = 0.827 \) for the XXZD model, which are identified as the KT transition. In figures 2(a) and (b), we plot the ground state fidelity per lattice site, \( d(\Delta_1, \Delta_2) \), for the spin 1/2 XXZ model and the spin 1 XXZD model (with a fixed \( J_z = -1/2 \)). We have chosen \( \Psi(\Delta_2) \) \((\Psi(D_2))\) as a reference state, with \( \Delta_2 = 0 \) \((D_2 = -0.2)\), then \( d(\Delta_1, \Delta_2) \) \((d(D_1, D_2))\) is able to distinguish infinite degenerate ground states, with a (pseudo) phase transition point as a *catastrophe point* (which coincides with the pseudo transition point from the pseudo-order parameter for a given \( \chi \), within the accuracy). Note that, in the pseudo \( U(1) \) symmetry-broken phase, \( d(\Delta_1, \Delta_2) \) and \( d(D_1, D_2) \) take all the values between two lines, which are extreme values,

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8 For a discussion about the scaling of the von Neumann entropy with the truncation dimension \( \chi \), see [23].

9 The KT transition is just one of the instabilities of the Luttinger liquid. Another example is the Pokrovski–Talapov transition [24]. However, different characteristic behaviors are exhibited in the ground state fidelity per lattice site, as seen for the XX chain in an external magnetic field [12].

10 Our simulation result of \( d(\Delta_1, \Delta_2) \) for the XXZ model does not match the exact expression \( \ln d(\Delta_1, \Delta_2) = 1/2(\ln 2 - \ln(\sqrt{K(\Delta_1)/K(\Delta_2)} + \sqrt{K(\Delta_2)/K(\Delta_1)}) \), derived from the Luttinger liquid description, combined with the Bethe ansatz, \( K(\Delta) = \pi/(2(\pi - \arccos \Delta)) \) [15]. This is expected, since the Luttinger liquid only describes the low energy physics for the XXZ model, whereas \( d(\Delta_1, \Delta_2) \) captures the physics in both the low energy and high energy sectors.

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Figure 2. The ground state fidelity per lattice site $d(\Delta_1, \Delta_2)$ for the spin 1/2 XXZ model (a) and $d(D_1, D_2)$ for the spin 1 XXZD model (with a fixed $J_z = -1/2$) (b). Here, the truncation dimension $\chi$ takes 8, 16, 32, and 50, respectively.

We have chosen $\Psi(\Delta_2)$ ($\Psi(D_2)$) as a reference state, with $\Delta_2$ ($D_2$) in the $U(1)$ symmetry-broken phase $\Delta_2 = 0$ ($D_2 = -0.2$), then $d(\Delta_1, \Delta_2)$ ($d(D_1, D_2)$) is able to distinguish infinite degenerate ground states, with a (pseudo) phase transition point as a catastrophe point. Note that, in the pseudo $U(1)$ symmetry-broken phase, $d(\Delta_1, \Delta_2)$ and $d(D_1, D_2)$ take all the values between two lines, which are extreme values, as shown for each $\chi$, as a result of an artifact of the iMPS algorithm. In fact, all the degenerate ground states collapse into the genuine ground state as $\chi \to \infty$. Therefore, an essential signature of the KT transition is that a catastrophe point turns into an essential singularity if $\chi \to \infty$.

as shown for each $\chi$ in figures 2(a) and (b). This is again an artifact of the iMPS algorithm, since all the degenerate ground states collapse into the genuine ground state as $\chi \to \infty$. An essential signature of the KT transition is that a catastrophe point turns into an essential singularity if $\chi \to \infty$.

We have also computed the von Neumann entropy for the spin 1/2 XXZ model and the spin 1 XXZD model (with a fixed $J_z = -1/2$) (not shown here). It detects the QPTs (see footnote 8), but does not distinguish infinite degenerate ground states arising from a pseudo SSB for a given $\chi$.

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7. Conclusions

We have unveiled a numerical phenomenon—a pseudo SSB—which shares all the features of a genuine SSB in the context of the iMPS algorithm: first, infinite degenerate symmetry-breaking ground states are produced, each of which breaks the continuous symmetries of a quantum system; second, the symmetry breakdown results from a randomly chosen initial state. In addition, the extent to which a continuous symmetry group is broken may be quantified by a pseudo-order parameter that is scaled down to zero as the truncation dimension \( \chi \) tends to \( \infty \), in order to keep consistency with the Mermin–Wegner theorem. In this scenario, a Goldstone mode survives as a gapless excitation in the critical phase, implying that the Luttinger liquid may be characterized as a limiting case of the conventional symmetry-breaking order. That is, the long-range order vanishes when the truncation dimension becomes \( \infty \). It turns out that a pseudo SSB is reflected as a catastrophe point in the ground state fidelity per lattice site for quantum lattice systems undergoing the KT transition, for any finite choice of the truncation dimension \( \chi \); such a catastrophe point turns into an essential singularity if \( \chi \to \infty \).

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