Ground-state fidelity and Kosterlitz–Thouless phase transition for the spin-1/2 Heisenberg chain with next-to-the-nearest-neighbor interaction

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Abstract
The Kosterlitz–Thouless transition for the spin-1/2 Heisenberg chain with the next-to-the-nearest-neighbor interaction is investigated in the context of an infinite matrix product state algorithm, which is a generalization of the infinite time-evolving block decimation algorithm (Vidal 2007 Phys. Rev. Lett. 98 070201) to accommodate both the next-to-the-nearest-neighbor interaction and spontaneous dimerization. It is found that, in the critical regime, the algorithm automatically leads to infinite degenerate ground-state wavefunctions, due to the finiteness of the truncation dimension. This results in pseudo-symmetry spontaneous breakdown, which is reflected as a catastrophe point in the ground-state fidelity per lattice site. In addition, this allows the introduction of a pseudo-order parameter to characterize the Kosterlitz–Thouless transition. Our work demonstrates that the ground-state fidelity per lattice site is able to capture the Kosterlitz–Thouless transition, which is in sharp contrast to the fidelity susceptibility that fails to detect it.

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(Some figures may appear in colour only in the online journal)

1. Introduction
Quantum phase transitions (QPTs) [1] are one of the most intriguing research subjects in condensed matter physics. A QPT occurs at absolute zero due to quantum fluctuations in a variety of quantum many-body systems. In the conventional Landau–Ginzburg–Wilson paradigm, a phase transition accompanies spontaneous symmetry breaking (SSB) [2, 3] that is characterized by a local-order parameter. However, it has now become clear that not all QPTs fall into this category [4]. In fact, topological phase transitions do not involve any SSB. This even dates back to the Kosterlitz–Thouless (KT) transition [5], first discovered
for a two-dimensional classical XY model. Actually, the KT transition is ubiquitous in one-dimensional quantum systems. It describes the instability of the Luttinger liquid under a marginal perturbation. Normally, it is not an easy task to determine whether or not the KT transition occurs in a specific system, because there are pathological problems in analyzing the KT transition numerically. One of these problems is that the finite size scaling technique [6], which is successful for second-order QPTs [1, 4], cannot be applied to the KT transition [7], since there are logarithmic corrections from the marginal perturbation.

Recently, a novel approach to QPTs in quantum many-body lattice systems has been put forward [8–14], which is based on fidelity, a measure of quantum state distinguishability, in quantum information science. As argued in [9, 10], the ground-state fidelity per lattice site is able to capture quantum criticality underlying many-body physics in condensed matter. This fact, combining with a practical means to compute the ground-state fidelity per lattice site for infinite-size quantum lattice systems, makes it practical to investigate critical phenomena in quantum many-body systems. Coincidentally, recent developments in the context of the tensor network (TN) algorithms for translation-invariant quantum lattice systems offer such a practical means. Here, we mention the infinite matrix product state (iMPS) algorithm [15] in one spatial dimension and the infinite projected entangled-pair states [16] in two or higher spatial dimensions. These algorithms exploit the translation invariance of the system and parallelizability of a TN representation of quantum many-body wavefunctions, which provides an efficient way to classically simulate quantum many-body lattice systems.

In a previous work [17], we have succeeded in applying the fidelity per site approach to study the KT transition in both the one-dimensional spin-1/2 XXZ model and the spin-1 XXZ model with uniaxial single-ion anisotropy. The KT transition is reflected as a catastrophe point in the ground-state fidelity per lattice site. This results in the introduction of a novel concept—pseudo-SSB, offering a novel perspective to understand the KT transition, in the conventional Landau–Ginzburg–Wilson paradigm, from the iMPS representation. As such, it resolved the controversy regarding whether or not the ground-state fidelity is able to detect the KT QPTs. However, more work is needed to clarify if such an approach is applicable to the KT transition in other quantum many-body lattice systems. As argued in [13], the fidelity susceptibility is unable to detect the KT transition in a spin-1/2 Heisenberg chain with the nearest-neighbor coupling and next-to-the-nearest-neighbor coupling. Therefore, it is desirable to address exactly the same model to see if the ground-state fidelity per lattice site detects the KT transition, thus offering compelling evidence for the fact that our approach advocated in [17] is generic. This vividly illustrates an essential difference between the fidelity per site approach and the fidelity susceptibility approach.

In this paper, we propose an iMPS algorithm, a generalization of the infinite time-evolving block decimation algorithm [15], which allows us to accommodate both the next-to-the-nearest-neighbor interaction and spontaneous dimerization. It is found that, in the critical regime, the algorithm automatically leads to infinite degenerate ground-state wavefunctions, due to the finiteness of the truncation dimension. This results in pseudo-symmetry spontaneous breakdown, which is reflected as a catastrophe point in the ground-state fidelity per lattice site. In addition, this allows the introduction of a pseudo-order parameter to characterize the KT transition, which must be scaled down to zero in order to be consistency with the Mermin–Wagner theorem [18].

### 2. Matrix product state algorithm on an infinite-size one-dimensional lattice

Suppose the model Hamiltonian takes the form $H = \sum_{i} h^{[i,i+1,i+2]}$, with $h^{[i,i+1,i+2]}$ being the sum of the nearest-neighbor and the next-to-the-nearest-neighbor three-body Hamiltonian
fluctuations and geometric frustration, we choose four sequential sites \( (A, B, C, D) \) as a unit cell. Starting with a randomly chosen initial state \(|\Psi(0)\rangle\), which is not orthogonal to the ground state energy \( E_0 \), a ground-state wavefunction can be computed by the imaginary time evolution \( |\Psi(\tau)\rangle = \exp(-iH\tau)|\Psi(0)\rangle / ||\exp(-iH\tau)|\Psi(0)\rangle|| \) with \( \tau \to \infty \). To realize the imaginary time evolution operation, the imaginary time \( \tau \) is divided into many small slices \( \delta \tau = \tau/N \) to approximate the continuous time evolution by a sequence of small gates. Meanwhile, the time evolution operator is expanded to a product of evolution operators acting on a three-site gate: \( U_3 = \exp(-\delta J_{i,i+1,i+2})\delta \tau \) with \( \delta \tau \ll 1 \), as follows from the Suzuki–Trotter decomposition [19]. Any wavefunction admits an iMPS representation in a canonical form: attached to each site is a four-index tensor \( \Gamma^\alpha_\beta \) and at each bond is a diagonal matrix \( \lambda_n \), where \( n = A, B, C \) and \( D \). Here, \( s \) is a physical index, \( s = 1, \ldots, d \), with \( d \) being the dimension of the local Hilbert space. \( l \) and \( r \) denote the bond indices, \( l, r = 1, \ldots, \chi \), with \( \chi \) being the truncation dimension. For simplicity, we use \( \Gamma \) instead of \( \Gamma^\alpha_\beta \) in the text below.

The updating procedure for the tensors \( \Gamma \) and the diagonal matrices \( \lambda_n \) \((n = A, B, C, D)\) in the iMPS representation under the action of the three-site gate \( U_3 \) is visualized in figure 2. 

(a) Apply the three-site gate \( U_3 \) onto the iMPS tensors \( \Gamma_A, \Gamma_B \) and \( \Gamma_C \).

(b) Contract the tensors \( \lambda_D, \lambda_A, \lambda_B, \lambda_C \) into a single tensor and reshape the tensor into a bond-ordered 3-site matrix \( M \).

(c) Perform a singular value decomposition (SVD) to the matrix \( M \). After truncating and reshaping, we get the tensors \( M_1 \) and \( V_1 \) and the updated diagonal matrix \( \lambda_B \).

(d) Insert the identity resolution \( I = \lambda_B^{-1/2} \lambda_C \) on the right-hand side and contract the tensors \( V_1 \) and \( \lambda_C^{-1} \) to get the updated \( \Gamma_C \), as done in step (e).

(f) Contract \( M_1 \) and \( \lambda_B \) into a matrix and perform an SVD again, one gets the tensors \( V_2 \) and \( V_3 \) and the updated \( \lambda_A \).

(g) Insert the identity resolution again. 

(h) All the tensors \( \Gamma_A, \Gamma_B \) and \( \Gamma_C \) and the diagonal matrices \( \lambda_A \) and \( \lambda_B \) are updated. Shifting the action of the three-site gate \( U_3 \) one site each time and repeating four times, we are able to update the tensors under the imaginary time evolution of a slice \( \delta \tau \). Repeating the procedure until the ground-state energy per lattice converges, an approximate ground-state wavefunction is generated in the iMPS representation.

3. Model

Consider a spin-1/2 Heisenberg chain with the nearest-neighbor coupling \( J \) and next-to-the-nearest-neighbor coupling \( \delta J \). It is described by the Hamiltonian

\[
H = J \sum_{i=-\infty}^{\infty} (S_i^1 \cdot S_{i+1}^1 + \delta S_i^1 \cdot S_{i+2}^1),
\]

Figure 1. A sketch for the zigzag chain with the nearest-neighbor interaction \( J \) and next-to-the-nearest-neighbor interaction \( \delta J \). The parameter \( \delta \) represents the ratio between the couplings. The dash-line box indicates the unit cell.
where $\sigma_i^{[j]}$ are the spin-1/2 Pauli operators at the $i$th site. The system is equivalent to a zigzag chain as shown in figure 1. We set the nearest-neighbor anti-ferromagnetic coupling $J = 1$ as the energy scale and consider the ratio interval $0 \leq \delta \leq 0.5$. The system undergoes the KT transition at $\delta_c \sim 0.241$ [20]: the Luttinger liquid state for $\delta < \delta_c$ and the dimerized state for $\delta > \delta_c$ [21, 22], respectively. Actually, the KT transition accompanies a discrete $Z_2$ SSB in the dimerized phase.

4. Ground-state fidelity per lattice site

The ground-state fidelity per lattice site, $d(\delta_1, \delta_2)$, with $\delta$ being the control parameter, is defined as the scaling parameter: $F(\delta_1, \delta_2) \sim d(\delta_1, \delta_2)^N$, with $N$ being the total number of lattice sites and $F(\delta_1, \delta_2) \equiv |\langle \Psi(\delta_1) | \Psi(\delta_2) \rangle |$ between two ground-state wavefunctions $|\Psi(\delta_1)\rangle$ and $|\Psi(\delta_2)\rangle$. It characterizes how fast the fidelity $F(\delta_1, \delta_2)$ varies when the thermodynamic limit is approached [9, 10]. In fact, the ground-state fidelity per lattice site $d(\delta_1, \delta_2)$ may be regarded as a partition function per site of a classical statistical vertex lattice model defined on the same lattice. That explains why $d(\delta_1, \delta_2)$ is able to detect QPTs [23]. That is, the ground-state fidelity per lattice site exhibits singular behavior when the control parameter $\delta$ crosses a transition point $\delta_c$.

Figure 3 shows the ground-state fidelity per lattice site, $d(\delta_1, \delta_2)$, as a function of $\delta_1$, when $\delta_2$ is fixed, for the Heisenberg model with the nearest-neighbor coupling $J$ and next-to-the-nearest-neighbor coupling $3J$, for different values of the truncation dimension $\chi$. The iMPS simulation is performed for a randomly chosen initial state. It automatically induces degenerate ground-state wavefunctions, which break the $SU(2)$ symmetry in the Luttinger liquid phase and the $Z_2$ symmetry in the dimer phase.

In figure 3(a), the reference state $\Psi(\delta_2 = 0)$ is chosen in the pseudo-$SU(2)$ symmetry-broken phase. The ground-state fidelity per lattice site, $d(\delta_1, \delta_2)$, as a function of $\delta_1$, takes
Figure 3. The ground-state fidelity per lattice site, $d(\delta_1, \delta_2)$, for the spin-1/2 Heisenberg chain with the nearest-neighbor coupling $J$ and next-to-the-nearest-neighbor coupling $J\delta$. We have chosen $\Psi(\delta_2)$ as a reference state, with $\delta_1$ fixed in different phases: (a) $\delta_2 = 0$ in the pseudo-$SU(2)$ symmetry-broken phase. There is a catastrophe point in $d(\delta_1, \delta_2)$, which tends to disappear, when $\chi$ approaches $\infty$. (b) $\delta_2 = 0.4$ in the $Z_2$ symmetry-broken phase. A bifurcation point always exists whatever the truncation dimension $\chi$ we choose, as it should for a discrete $Z_2$ SSB. Therefore, the ground-state fidelity per lattice site, $d(\delta_1, \delta_2)$, is able to distinguish degenerate ground states, with a (pseudo)-critical point as a catastrophe (bifurcation) point. Here, we note that the catastrophe point is in exactly the same location as the bifurcation point for a given $\chi$.

Infinite many values lying between two extremes, as a consequence of infinite degenerate ground states, if $\delta_1$ is in the pseudo-$SU(2)$ symmetry-broken phase. In contrast, when $\delta_1$ is in the $Z_2$ symmetry-broken phase, $d(\delta_1, \delta_2)$ yields just one value. Thus, a catastrophe point occurs, which is defined as a pseudo-transition point $\delta_1^c$. With increasing $\chi$, the difference between two extreme values of $d(\delta_1, \delta_2)$ decreases. Therefore, the catastrophe point tends to disappear when $\chi$ goes to infinity, implying that degenerate ground states arise from the finiteness of the truncation dimension, an artifact of the iMPS algorithm. In fact, all the degenerate ground states should collapse into the genuine ground state as $\chi$ approaches $\infty$, as required to keep consistency with the Mermin–Wagner theorem; no continuous symmetry is spontaneously broken in one-dimensional quantum systems. However, the critical point $\delta_1^c$ may be determined by performing an extrapolation with respect to a few reasonably small $\chi$s, as advocated in our previous work [17].

In figure 3(b), the reference state $\Psi(\delta_2 = 0.4)$ is chosen in the $Z_2$ symmetry-broken phase. Here, the ground-state fidelity per lattice site, $d(\delta_1, \delta_2)$, as a function of $\delta_1$, takes two different values, as a consequence of two degenerate ground states arising from spontaneous dimerization, if $\delta_1$ is in the $Z_2$ symmetry-broken phase. In contrast, when $\delta_1$ is in the pseudo-$SU(2)$ symmetry-broken phase, $d(\delta_1, \delta_2)$ yields just one value. Thus, a bifurcation point occurs in the ground-state fidelity per lattice site. However, the bifurcation does not vanish, when $\chi$ approaches $\infty$. Instead, it tends to saturate when $\chi$ increases. This is expected, since the bifurcation point arises from the discrete $Z_2$ SSB. Here, we note that the catastrophe point is in exactly the same location as the bifurcation point for a given $\chi$.

Therefore, we conclude that, for a finite truncation dimension $\chi$, the iMPS algorithm enables us to yield infinitely many degenerate ground states in the pseudo-$SU(2)$ symmetry-broken phase and two degenerate ground states in the $Z_2$ symmetry-broken dimer phase. In addition, the ground-state fidelity per lattice site, $d(\delta_1, \delta_2)$, is able to distinguish two (infinitely many) degenerate ground-state wavefunctions with a reference state in the $Z_2$ (pseudo-$SU(2)$) symmetry-broken phase. This implies that the KT transition is generic, with its critical point accurately determined by computing the ground-state fidelity per lattice site, $d(\delta_1, \delta_2)$, with a
Figure 4. The pseudo-local-order parameter $O_\chi$ as a function of $\delta$. The iMPS simulation is performed for a randomly chosen initial state. An extrapolation of the pseudo-critical point $\delta c^\chi$ is performed for pseudo-transition points, at which the pseudo-order parameter becomes zero, yielding the KT transition point $\delta_c = 0.2418$ in the right-top inset. The right-bottom inset shows that, in the critical phase, the pseudo-order parameter is scaled down to zero according to $O_\chi = a\chi^{-b}(1 + c\chi^{-1})$, with $a = 0.5993$, $b = 0.6150$ and $c = 1.0379$, to keep consistency with the Mermin–Wagner theorem.

5. Pseudo-order parameter

As is well known, the iMPS algorithm yields the best approximation to a ground-state wavefunction for a lattice system with a gap. However, for a gapless system with continuous symmetry, if the truncation dimension $\chi$ is finite, the iMPS algorithm automatically produces infinitely many degenerate ground states from a randomly chosen initial state [17], each of which breaks the continuous symmetry. That is, a numerical phenomenon occurs, which shares all the features of an SSB resulting from random perturbations. Such a pseudo-symmetry-broken order may be quantified by introducing a pseudo-local-order parameter, which may be read off from a reduced density matrix on a local area [23]. However, this phenomenon is in contradiction with the Mermin–Wagner theorem, which states that no continuous symmetry is spontaneously broken for quantum systems in one spatial dimension [18]. To resolve this apparent contradiction, one has to require that the pseudo-local-order parameter must be scaled down to zero, when the truncation dimension $\chi$ goes to $\infty$. We emphasize that both pseudo-SSB and pseudo-local-order parameter arise from the artifact of the iMPS algorithm, in sharp contrast with a genuine SSB and a local-order parameter.

For the Heisenberg model with the nearest-neighbor coupling $J$ and next-to-the-nearest-neighbor coupling $J\delta$, the pseudo-local-order parameter may be chosen as $O_\chi = \sqrt{(S_x)^2 + (S_y)^2 + (S_z)^2}$ for the truncation dimension $\chi$. The pseudo-local-order parameter $O_\chi$ is plotted as a function of $\delta$ in figure 4. The iMPS simulation is performed for a randomly chosen initial state, with the truncation dimension $\chi$ to be 4, 8, 16, 32 and 64, respectively. Note that $O_\chi$ is zero in the $Z_2$ symmetry-broken phase, but nonzero in the pseudo-$SU(2)$ symmetry-broken phase, due to the finiteness of the truncation dimension $\chi$. However, this is nothing but an artifact of the iMPS algorithm. Remarkably, one may take moderate computational cost. We emphasize that an essential signature of the KT transition is a catastrophe point, which tends to vanish and turns into an essential singularity if $\chi$ approaches $\infty$ [17].
advantage of this artifact to locate a critical point $\delta c$. Note that an extrapolation with respect to $\chi$ may be performed for the pseudo-phase-transition points $\delta c$, at which the pseudo-local-order parameter becomes zero. In the right-top inset of figure 4, the KT transition point $\delta c = 0.2418$ is determined from such an extrapolation, which is comparable with $\delta c = 0.2411$ from the level spectroscopy analysis [20]. Here, we require that the pseudo-local-order parameter must vanish, when $\chi$ goes to $\infty$, to keep consistency with the Mermin–Wagner theorem. Therefore, a fitting function $O_\chi = a\chi^{-b}(1 + c\chi^{-1})$ is chosen, with $a = 0.5993$, $b = 0.6150$ and $c = 1.0379$, as shown in the right-bottom inset in figure 4. This ensures that, when $\chi \to \infty$, all the degenerate ground states collapse into the genuine ground state.

6. Conclusion

We have investigated the KT transition for the spin-1/2 Heisenberg chain with the nearest-neighbor coupling $J$ and next-to-the-nearest-neighbor coupling $J\delta$ in the context of an iMPS algorithm. The latter is a generalization of the infinite time-evolving block decimation algorithm to accommodate both the next-to-the-nearest-neighbor interaction and spontaneous dimerization. It is demonstrated that, in the critical regime, the algorithm automatically leads to infinitely many degenerate ground-state wavefunctions, due to the finiteness of the truncation dimension. This results in pseudo-symmetry spontaneous breakdown, reflected as a catastrophe point in the ground-state fidelity per lattice site. In addition, this allows the introduction of a pseudo-local-order parameter to characterize the KT transition, which scales down to zero when $\chi$ approaches infinity. Our work offers compelling evidence that the ground-state fidelity per lattice site is able to detect the KT transition, in contrast to the fidelity susceptibility approach.

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