Phase diagram of the spin-1/2 Heisenberg alternating chain in a magnetic field

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By using the infinite time-evolving block decimation, we study quantum fidelity and entanglement entropy in the spin-1/2 Heisenberg alternating chain under an external magnetic field. The effects of the magnetic field on the fidelity are investigated, and its relation with the quantum phase transition (QPT) is analyzed. The phase diagram of the model is given accordingly, which supports the Haldane phase, the singlet-dimer phase, the Luttinger liquid phase and the paramagnetic phase. The scaling of entanglement entropy in the gapless Luttinger liquid phase is studied, and the central charge $c = 1$ is obtained. We also study the relationship between the quantum coherence, string order parameter and QPTs. Results obtained from these quantum information observations are consistent with the previous reports.

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I. INTRODUCTION

Quantum phase transition (QPT) is a purely quantum process occurring in strongly correlated many-body systems at absolute zero temperature due to quantum fluctuations [1]. The spin chains attract a lot of attention since they give rise to many exotic properties in the ground state, such as bond alternating spin-1/2 Heisenberg chain [2–9]. A number of compounds are discovered whose properties can be explained by invoking bond alternating chains. LiInCr4O8 was found to be spin-3/2 breathing pyrochlore antiferromagnet, which is an alternating array of small and large tetrahedra [10]. Recently, it is reported that the results from the dimer anisotropic XYZ model are relevant to a large number of quasi-one dimensional magnets [11]. In history, Bulaevski predicted that a spin gap exists in the nonuniform antiferromagnetic (AFM) spin chains [12]. Kohmoto found the existence of the Haldane phase synonymous with hidden $D_2$ symmetry breaking in the AFM-ferromagnetic (FM) bond alternating spin-1/2 Heisenberg chain [13]. Furthermore, it was pointed out that isotropic $S = 1/2$ Heisenberg chain with alternating AFM and FM couplings can be mapped onto the isotropic $S = 1$ AFM Heisenberg chain when the FM couplings tend to infinity [14]. The compounds like CuGeO3 [15] exhibiting spin-Peierls transitions belong to AFM-AFM bond alternating class, and DMACuCl3 [16] was claimed to fall into the $S = 1/2$ AFM-FM bond alternating class. Additionally, the quantum simulation using ultracold atoms systems [17,19] and trapped polariton condensates [20] has made great progress in creating interesting quantum models motivated by solid-state physics. Geometrically frustrated magnets such as zigzag chains can be designed and tuned by the depth of the optical lattice, and thus nonuniform configurations in the ground state can be anticipated.

The magnetic phase transitions induced by applying a magnetic field in the low-dimensional magnets have attracted much interest recently from both experimental and theoretical points of view. When the magnetic interactions cannot be satisfied simultaneously owing to the existing competing orders, the magnetic systems become fertile ground for the emergence of exotic states. The ground-state magnetization plateaus appearing in polymerized Heisenberg chains under external magnetic fields was investigated, and the phase diagram of AFM bond alternating spin chain in homogeneous magnetic fields was presented [21,22]. Moreover, the effects of temperature, magnetic field and dimerized interaction on the spin and heat transport in dimerized Heisenberg chains in a magnetic field are studied. It is noted that the spin and heat conductivity show different behaviors in different phases [23]. For alternating spin-1/2 chains with anisotropic AFM-FM coupling under a transverse magnetic field, two successive phase transitions, i.e., from Haldane phase to stripe AFM phase and from stripe AFM phase to polarized paramagnetic phase, have been identified to be Ising type [24]. The magnetization state and magnetic structure can be revealed through common techniques like neutron diffraction measurements and synchrotron X-ray scattering [25,26]. However, the phase boundary of the spin-1/2 Heisenberg AFM-FM bond alternating chain in a magnetic field is still not clear, and needs to be discussed further. Fortunately, with the development of quantum information, various information measures, e.g., quantum coherence, entanglement entropy, and fidelity, can help us to study quantum critical phenomena in spin chains. It is found that the quantum critical points can be well characterized by both the ground-state entanglement and fidelity on large system [27,34]. In this paper we study the entanglement,
been shown that the dimerized XX model is equivalent to anisotropic XY model in given parity blocks [35]. It is more straightforward to see the equivalence between them in the fermionic form:

\[
H_{DXX} = \sum_{i=1}^{N/2} \left( \frac{1}{2} (c_{2i}^+ c_{2i+1} + \lambda c_{2i}^+ c_{2i+1}^+ + h.c.) \right) + \sum_{i=1}^{N} \left( \frac{B}{2} (1 - 2c_i^+ c_i) \right). \tag{2}
\]

Then, we use the local mapping under the assumption of even \( N \) and periodic boundary condition:

\[
c_j^+ = \frac{1}{2} \left[ ia_{j+1}^+ + a_j^+ - (-1)^j (ia_{j+1} + a_j) \right], \tag{3}
\]

and thus Eq.\,(2) can be transformed into a generalized anisotropic model:

\[
H_{AXX} = \sum_{j=1}^{N} \left( J_h a_j^+ a_{j+1} + J_p a_j^+ a_{j+1}^+ + h.c. \right) + \sum_{j=1}^{N} \frac{iB}{2} \left[ a_j^+ a_{j+1} - (-1)^j a_{j+1}^+ a_{j+1} + h.c. \right]. \tag{4}
\]

where \( J_h = (1 + \lambda)/4, \ J_p = (\lambda - 1)/4 \). Eq.\,(4) can be traced back to the spin version:

\[
H = \sum_{j=1}^{N} \left( \lambda S_j^x S_{j+1}^x + S_j^y S_{j+1}^y \right) + B \sum_{j=1}^{N/2} (S_{2j-1}^z S_{2j}^z - S_{2j}^z S_{2j+1}^z). \tag{5}
\]

For \( B = 0 \) the QPT occurring at \( \lambda = 1 \) for the dimerized chain shares the same properties with the transition which occurs at \( \lambda = 1 \) for the anisotropic XY chain separating the \( x \)-component phase from the \( y \)-component Néel phase. In the case of \( \lambda = 1 \) dimerized XX model corresponds to the uniform XX chain. In the opposite limit \( \lambda = 0 \) one arrives at a collection of isolated (uncoupled) XX dimers. \( B \) term in Eq.\,(5) favors period-4 configurations \( \uparrow \downarrow \downarrow \uparrow \downarrow \ldots \) or \( \downarrow \uparrow \downarrow \uparrow \downarrow \ldots \), competing with \( x \)-component and \( y \)-component Néel orderings. The generic features of the spin-Peierls systems are analytically discussed in detail by Taylor and Müller [36]. The details can be referred to Appendix \( \text{A} \).

As we know, it is difficult to diagonalize the Hamiltonian Eq.\,(1) when \( \Delta \neq 0 \). The finite-size density matrix renormalization group (DMRG) would be the effective method to obtain the ground-state wavefunctions approximately [37 35]. In this version of DMRG, an open chain is grown iteratively by adding two sites at a time to the center of the spin chain, and up to the sizes \( N = 400 \). Then, we perform four sweepings, and the maximum number of the eigenstates kept is \( m = 200 \) during the processing. Such truncation guarantees that the converging error is smaller than \( 10^{-7} \). With this accurate
calculation, we can precisely analyze the QPTs through various theoretic measures.

A QPT taking place in this class of systems has been thoroughly investigated in the thermodynamic limit. However, both experimental and theoretical difficulties have boosted a high interest in finite-size systems, which show the forerunners of the points of QPT of the thermodynamic systems. In general, finite-size systems would exhibit many energy level crossings between physical and unphysical states. As a consequence, diverse theoretic measures would have some jumps. In order to avoid the finite-size effects, we also implement the infinite time-evolving block decimation (iTEBD) [39, 40], which can be used to compute the ground-state wavefunctions for an infinite-size lattice in one or two dimensions with translational invariance. It can help us directly address physical quantities in the thermodynamic limit with high quality. Given a large bond dimensions χ, the ground-state wavefunctions based on the matrix product state representations can be obtained by applying imaginary-time evolution gates exp(−τh) on a given initial random state |ψ(0)⟩, until the latter converges to the variational ground state. Here h is the local Hamiltonian, which is composed of two-site coupling terms on an odd bonds h_{2i−1,2i} or even bonds h_{2i,2i+1}, and τ is the Trotter step length. In practice, we start from τ = 0.1 and gradually reduce it by τ = τ/10, and break the loop until τ < 10−9. In the paper, χ = 50 is adopted, and we check our codes with the case λ = 1, B = 0, which is equal to well-known Heisenberg chain. The ground-state energy we obtain is E_0 = −0.443143049, which is very close to the exact diagonalization result E = 1/4 − ln(2) = −0.4431471805, and the error is smaller than 5.0 × 10−6.

As the external parameter varies across a critical point, the ground-state wavefunction undergoes a sudden change in the wake of QPT, accompanied by a rapid alteration in a variety of quantum measurements. Fidelity is one of the most effective measurements, which can detect the critical points [41,43]. It measures the similarity between the two closest states as the external parameter such as κ is tuned, which is defined as \( F_N(\kappa_1, \kappa_2) = |\langle \psi(\kappa_1) | \psi(\kappa_2) \rangle| \) in finite-size systems. In the thermodynamic limit, the ground-state fidelity per site

\[
d(\kappa_1, \kappa_2) = \lim_{N \to \infty} F_N^{1/N}(\kappa_1, \kappa_2)
\]

can be calculated easily in iTEBD by transfer matrix [43]. The fidelity \( d(\kappa_1, \kappa_2) \) should be equal to one when \( \kappa_1 = \kappa_2 \), and QPTs may be detected through singularities exhibited in \( d(\kappa_1, \kappa_2) \). Meanwhile, the concurrence is chosen as a measure of the pairwise entanglement between two qubits [44]. The concurrence C is defined as

\[
C(\rho_{12}) = \max\{\beta_1 - \beta_2 - \beta_3 - \beta_4, 0\},
\]

where the quantities \( \beta_i (i = 1, 2, 3, 4) \) are the square roots of the eigenvalues of the operator \( \sigma_i^{x_1} \otimes \sigma_i^{y_2} \rho_{12}^{\dagger} (\sigma_i^{x_1} \otimes \sigma_i^{y_2}) \) and in descending order. The case of \( C = 1 \) corresponds to the maximum entanglement between the two qubits, while \( C = 0 \) means that there is no entanglement between the two qubits. The entanglement entropy is used as a measure of the bipartite entanglement. If \( \psi \) is the ground state of a chain of N qubits, a reduced density matrix of contiguous qubits from 1 to L can be written as \( \rho_L = Tr_{N-L}(|\psi\rangle \langle \psi|) \). The bipartite entanglement between the right-hand L contiguous qubits and the rest of the system can be measured by the entropy

\[
S_L(\rho_{1..L}) = -Tr(\rho_L \log_2 \rho_L).
\]

One of the basic properties of the block entanglement entropy for a pure state can be given by \( S_L = S_{N-L} \), since the spectrum of the reduced density matrix \( \rho_L \) is the same as that of \( \rho_{N-L} \) following from the Schmidt decomposition. This property implies the entanglement entropy is not extensive and boils down to a celebrated area law for non-critical ground states or finite temperature system, which states the leading term of the entanglement

FIG. 2. Ground state fidelity per site \( d(B_1, B_2) \) for the model with different alternating interactions (a) \( \lambda = 0.5 \) (b) \( \lambda = -1 \).
entropy is proportional to the boundary area between \( L \) and \( N - L \) qubits. Note that the area law is violated for highly excited states and for ground state of gapless systems.

III. RESULTS

The ground-state phase diagram of the Hamiltonian Eq. (1) for \( \Delta = 1 \) is shown in Fig. 1. Note that the phase diagram on \( B-\lambda \) plane has been shown in Refs. [22, 23] for \( \lambda > 0 \). We calculated the fidelity per site to check our codes, which is shown in Fig. 2(a). It is seen that \( d(B_1, B_2) = 1 \) when \( |\psi(B_1)\rangle, |\psi(B_2)\rangle \) are both in the dimerized phase or both in the paramagnetic phase at the same time. The two pinch points which mean the critical points can be identified as \( B_{c1} = 0.64, \ B_{c2} = 1.53 \). The values agree with the results obtained by the spin gap \[ 2 \ [45, 46]. When \( B_{c1} < B < B_{c2} \), the model will be in the Luttinger liquid phase, which is gapless. We also show the phase diagram for \( \lambda < 0 \). It is obvious that the model would be in Haldane phase for \( B = 0 \) and paramagnetic phase with large magnetic field. The Luttinger liquid phase separates these phases for intermediate \( B \). The critical points between them can also be portrayed by the fidelity. The result is shown in Fig. 2(b). The two pinch points can be found \( B_{c3} = 0.61, \ B_{c4} = 1.00 \) for \( \lambda = -1 \).

FIG. 4. The string order parameter \( O^\text{even} _x (r) \) is plotted as a function of the magnetic field \( B \) and site distance \( r \) for with \( \lambda = -1 \).
Luttinger liquid phase. When \( \text{SOP} \) decays suddenly, indicating the system changes to 0 when \( 0 < B < 1 \). Here we set \( i \) most one, and has little change with the distance \( r \) where the density matrix \( \rho \) describes a quantum state, \( K \) plays a role of an observable, and \( [.,.] \) denotes the commutator. The WSYI shows the capability of diagnosing the QPT in the anisotropic XY chain \([52]\). Similar with the entanglement entropy, the quantum coherence is shown in Fig. 6. All the phase transitions can be identified by divergences or discontinuity of coherence for even bonds and odd bonds.

\[
C_i(\rho) = \sum_{i \neq j} (i|\rho|j).
\]  

Moreover, the local quantum coherence and the local quantum uncertainty, based on Wigner-Yanase skew information (WSYI), given by \([61]\)

\[
I(\rho, K) = -\frac{1}{4} \text{Tr}([\rho, K]^2),
\]

where the density matrix \( \rho \) describes a quantum state, \( K \) plays a role of an observable, and \( [.,.] \) denotes the commutator. The WSYI shows the capability of diagnosing the QPT in the anisotropic XY chain \([52]\). Similar with the entanglement entropy, the quantum coherence is shown in Fig. 6. All the phase transitions can be identified by divergences or discontinuity of coherence for even bonds and odd bonds.

**IV. CONCLUSIONS**

By using the infinite time-evolving block decimation, the ground-state properties of the spin-1/2 Heisenberg...
alternating chain in a magnetic field are calculated with very high accuracy. We numerically investigate the effects of magnetic field on the fidelity, which measures the similarity between two states, and then analyze its relation with the quantum phase transitions (QPTs). QPTs are intuitively accompanied by an abrupt change in the structure of the ground-state wave function, so generally a pinch point of the fidelity indicates a QPT and the location of the pinch point denotes the critical point. Based on the above analysis, we obtain the phase diagram. This model supports the Haldane phase, the singlet-dimer phase, the Luttinger liquid and the paramagnetic phase. In the Luttinger liquid phase, we study the scaling of the entanglement entropy with the subsystem size $L$, and identified the central charge $c = 1$. We also study the quantum coherence, whose anomalies detect all the phase transitions therein. In summary, conclusions drawn from these quantum information observables agree well with each other.

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Appendix A: Exact solution of dimerized XX model

Consider a chain of spin-1/2 operators interacting antiferromagnetically with their nearest neighbors, given by

\[ H = \sum_{i=1}^{N/2} J(S_{2i-1}^y S_{2i}^x + S_{2i-1}^x S_{2i}^y) + \lambda(S_{2i}^x S_{2i+1}^x + S_{2i}^y S_{2i+1}^y) \]
\[- B \sum_{i=1}^{N} S_i^z. \]  \hspace{1cm} (A1)

The dimerized XX model corresponds to \( \Delta = 0 \) in Eq. (4). The Hamiltonian (A1) can be exactly diagonalized following the standard procedure for 1D systems. In terms of the raising and lowering operators for spins,

\[ S_i^+ = S_i^x + iS_i^y, \quad S_i^- = S_i^x - iS_i^y, \]  \hspace{1cm} (A2)

The Hamiltonian (A1) then takes the form:

\[ H = \sum_{i=1}^{1/2} \left( \frac{S_{2i-1}^+ S_{2i}^- + S_{2i-1}^- S_{2i}^+}{} + \frac{\lambda}{2} (S_{2i}^+ S_{2i+1}^- + S_{2i}^- S_{2i+1}^+) \right) + B S_i^z. \]  \hspace{1cm} (A3)

The Jordan-Wigner transformation maps explicitly between quasispin operators and spinless fermion operators by

\[ S_j^+ = \exp \left[ i \pi \sum_{i=1}^{j-1} c_i^c_i c_j \right] c_j = \prod_{i=1}^{j} (2S_i^c)c_j, \]
\[ S_j^- = \exp \left[ -i \pi \sum_{i=1}^{j-1} c_i^c_i c_j \right] c_j = \prod_{i=1}^{j} (2S_i^c)c_j, \]
\[ S_j = 1/2 - c_j^c_j, \]  \hspace{1cm} (A4)

where \( c_j^c_j \) are annihilation and creation operators of spinless fermions at site \( j \), which obey the standard anticommutation relations, \( \{c_i, c_j\} = 0, \{c_i^c, c_j\} = \delta_{ij} \). By substituting Eq. (A4) into Eq. (A1), we find

\[ H = \sum_{i=1}^{N/2} \left[ \frac{1}{2} (c_{2i}^+ c_{2i} + c_{2i} c_{2i+1}^+) + \frac{\lambda}{2} (c_{2i}^c c_{2i+1} + c_{2i} c_{2i+1}^c) \right] + \sum_{i=1}^{N} \frac{B}{2} (1 - 2c_i^c c_i). \]  \hspace{1cm} (A5)

Next, utilizing translational invariance, discrete Fourier transformation for plural spin sites is introduced by

\[ c_{2j-1} = \sqrt{\frac{2}{N}} \sum_k e^{-ik} a_k, \quad c_{2j} = \sqrt{\frac{2}{N}} \sum_k e^{-ik} b_k, \]  \hspace{1cm} (A6)

with the discrete momentums as

\[ k = \frac{2n\pi}{N}, \quad n = -\frac{N}{2}, -\frac{N}{2} - 1, \ldots, \frac{N}{2} - 1. \]  \hspace{1cm} (A7)

Let’s proceed with diagonalization of the dimerized XX model. We rewrite,

\[ H = \sum_k (-\frac{1}{2} - \frac{\lambda}{2} e^{ik}) b_k a_k^+ + \sum_k (\frac{1}{2} + \frac{\lambda}{2} e^{ik}) b_k^c a_k^c \]
\[ + \sum_k \frac{B}{2} (1 - 2a_k^c a_k) + \sum_k \frac{B}{2} (1 - 2b_k^c b_k). \]  \hspace{1cm} (A8)

Defining

\[ \Lambda_k = \frac{1}{2} + \frac{\lambda}{2} e^{ik}, \]  \hspace{1cm} (A9)

then Eq. (A8) can be rewritten as

\[ H = \sum_k \left( a_k^+ b_k^c + \Lambda_k^* b_k^c a_k^c \right) + \sum_k B (1 - a_k^c a_k - b_k^c b_k). \]  \hspace{1cm} (A10)

Then we write the Hamiltonian in the matrix form:

\[ H = \sum_k \left( a_k^+ b_k^c \right) \left( -B \Lambda_k \right) \left( a_k^c b_k \right) + \sum_k B. \]  \hspace{1cm} (A11)

The eigenspectra can be obtained as:

\[ \varepsilon_{\pm,k} = \pm |\Lambda_k| - B. \]  \hspace{1cm} (A12)

Consequently, the Hamiltonian can be written in the diagonal form:

\[ H = \sum_k \left[ \varepsilon_{+,k}(\gamma^+_1 \gamma^-_1 - 1) + \varepsilon_{-,k}(\gamma^+_2 \gamma^-_2 - 1) \right], \]  \hspace{1cm} (A13)

where

\[ \varepsilon_{+,k} = \frac{1}{2} \sqrt{1 + \lambda^2 + 2\lambda \cos k - B}, \]
\[ \varepsilon_{-,k} = -\frac{1}{2} \sqrt{1 + \lambda^2 + 2\lambda \cos k - B}. \]

As a magnetic field is turned on, the one-particle spectrum will simply moves to higher energies with its shape unchanged. Since the \( \varepsilon_{-,k} \) is always negative, the gap closing can be identified by \( \partial \varepsilon_{+,k}/\partial k = 0 \), which suggests that the boundaries are described by \( B = |1 + \lambda|/2 \) for \( k = 0 \) and \( B = |1 - \lambda|/2 \) for \( k = \pi \) as shown in Fig. 7.