Entanglement, purity and fidelity in the anisotropy (1/2, 1) mixed-spin system

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\textbf{A B S T R A C T}

We study entanglement, purity and fidelity in the anisotropy (1/2, 1) mixed-spin Heisenberg chain. We find that negativity, as a measure of entanglement, displays a dip at the SU(2) isotropic point of the system, which is in contrast to the peak appearance of concurrence in the spin-1/2 XXZ chain. Moreover, at the isotropic point, purity gives a minimum, while the mixed-state fidelity susceptibility emerges a maximum.

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\section{Introduction}

Entanglement is a key concept in quantum information theory [1]. Purity, a measurement of the mixedness of system, is always associated with entanglement. In practice, due to decoherence, it is interesting to investigate entanglement and purity in mixed states as well as their relations [2--5]. One can use them to characterize the basic properties of the states of systems [6]. In quantum information theory, there is another concept closely connected to entanglement, which is called fidelity [1]. It is first proposed as a tool to describe the stability of a quantum system to the external perturbations [7], and it also characterizes quantum entanglement [8] to some extent. Recently, these concepts are being applied to study the properties of quantum many-body systems. For example, entanglement [9--15] and fidelity [16--23] are employed to indicate quantum phase transitions (QPTs) of the systems.

Stimulated by the above works, in this paper, we will employ the concepts of entanglement, purity and fidelity to investigate the ground-state properties of the one-dimensional mixed-spin XXZ Heisenberg chain, whose critical behaviors have been studied by Alcaraz and Malvezzi [24] using finite-size calculations and conformal invariance. The system under consideration consists of two kinds of spins, spin-1/2 and -1, alternating on a ring, with its Hamiltonian given by

\begin{equation}
H_0 = \sum_{l=1}^{L} (s_{l} \cdot s_{l+1} + s_{l+1} \cdot s_{l+2}) + (\Delta - 1) \sum_{l=1}^{L} (s_{l}^z \cdot s_{l+1}^z + s_{l+1}^z \cdot s_{l+2}^z),
\end{equation}

where $s_{l}$ and $s_{l}$ are spin-1/2 and spin-1 operators at the $l$th site (each site contains two kinds of spins), respectively. $L$ denotes the system size, and we only consider the cases $L$ is even in this study. The exchange interactions exist only between nearest
neighbors, and they are of the same strength, which is set to unity. $\Delta$ is the anisotropy parameter and in this paper only the region $\Delta \geq 0$ is considered. In addition, we adopt the periodic boundary condition in the system.

In the work of Alcaraz and Malvezzi [24], they found that, in the regime $-1 \leq \Delta < 1$, the ground state of the system is single or double degenerate, and the model is in a gapless phase. However, in the Ising regime $\Delta > 1$, the ground states are of twofold degeneracy, and the ground states have a finite energy gap in the limit of $L \to \infty$. Special properties can be expected at the isotropic point, i.e., $\Delta = 1$. At this point, the system exhibits ferrimagnetic order and the ground state is highly degenerate with the degeneracy related to the system size. For example, in the $(1/2, 1)$ mixed-spin case, the ground state has the degeneracy of $1 + L/2$ at the isotropic point. Therefore, the position $\Delta = 1$ is a critical point indicating the reconstruction of the energy spectrum of the system. In this work, it is expected that the three concepts, entanglement, purity and fidelity, which are closely associated with the system structure, will present special behaviors at the critical point.

For the ground states of the system under consideration, its degeneracy is not fixed as $\Delta$ varies, so it is difficult to write an exact and convenient form of the ground states. To solve this problem, in our paper, the ground state is approximately represented by the thermal state at low enough temperature. The state at thermal equilibrium can be described by the Gibb’s density operator $\rho(T) = \exp(-\beta H)/Z$, where $\beta = 1/k_B T$, $k_B$ is the Boltzmann’s constant, and $Z = \text{Tr}\{\exp(-\beta H)\}$ is the partition function. When the temperature is low enough, the thermal state gives the mixture of all the degenerate ground states with equal probability. Although this method is not an absolutely exact one, the state $\rho(T)$ can still well manifest the properties of the ground states [25].

The paper is organized as follows. In Section 2, we investigate the entanglement between the nearest-neighbor sites, and present the special properties of entanglement at the isotropic point. In Section 3, we study the purity and fidelity of the ground states of the system. The fidelity susceptibility shows a remarkable peak at the isotropic point. The conclusion will be given in Section 4.

2. Entanglement of two nearest-neighbor sites

For the case of higher spins, a non-entangled state has a necessarily positive partial transpose according to the Peres–Horodecki criterion [26]. In the case of two spin halves, and the case of $(1/2, 1)$ mixed spins, fortunately, a positive partial transpose is also sufficient for a separate state. This allows us to investigate the entanglement features of the mixed-spin systems. The quantitative Peres–Horodecki criterion was developed by Vidal and Werner [27]. They presented a measure of entanglement called negativity that can be computed efficiently, and it does not increase under local manipulations of the system. The negativity of a two-spin state $\rho$ is defined as

$$\mathcal{N}(\rho) = \sum_i |\mu_i|,$$

where $\mu_i$ is the negative eigenvalue of $\rho^{T_1}$, and $T_1$ denotes the partial transpose with respect to the first spin subsystem. The negativity $\mathcal{N}$ is related to the trace norm of $\rho^{T_1}$ via

$$\mathcal{N}(\rho) = \frac{||\rho^{T_1}|| - 1}{2},$$

where the trace norm of $\rho^{T_1}$ is equal to the sum of the absolute values of the eigenvalues of $\rho^{T_1}$. In this paper, we will use the concept of negativity to study the entanglement in $(1/2, 1)$ mixed-spin systems.

We numerically study the entanglement of two nearest-neighbor sites with two kinds of spins denoted by 1 and 2 according to the following steps. Firstly, we derive the reduced density matrix $\rho_{1,2}$ by tracing out all other spin degrees of freedom. Subsequently, we make partial transpose $T_1$ for the state $\rho_{1,2}$ and obtain the negativity $\mathcal{N}(\rho_{1,2})$ finally.

Fig. 1 displays the negativity in the mixed-spin system versus parameter $\Delta$ for different system sizes, $L = 4, 6, 8$. It is evidently found that with the increasing of $\Delta$, the negativity undergoes a dip at the isotropic point $\Delta = 1$. This is because the SU(2) symmetry of the mixed-spin system at $\Delta = 1$ induces high degeneracy of the ground states. As a result, the mixed degree of the ground states is increased (see Fig. 3). This weakens the quantum coherence so that the entanglement at this point is reduced.

The inset of Fig. 1 shows the crossing of ground-state energy levels occurs at the SU(2) point. This gives an interpretation of the degeneracy change from the viewpoint of energy structure. In other words, the special behaviors of the ground-state entanglement shown in Fig. 1 reflect the configuration variance of the system at the point $\Delta = 1$.

It should be noted that, since we use the exact diagonalization method here to numerically obtain the reduced density matrix $\rho_{1,2}$, only small-size systems are considered. Nevertheless, small-size systems can also well exhibit the entanglement properties of large-size systems [25]. For example, in Fig. 1, the curves correspond to $L = 6$ and $L = 8$ tend to be close, which provide a reasonable indication that the entanglement in the $L = 8$ system reflects enough information of entanglement in the large-site systems. Generally, it is difficult to simulate a spin chain of large length, thus a natural idea is to study small systems. Fortunately, small-size systems can also well exhibit the entanglement properties of large-size systems. For instance, in the anisotropic spin-1/2 Heisenberg model with a large number (as large as 1280) of qubits, the pairwise entanglement shows a maximum at the isotropic point [13]. This feature was already shown in a small system with periodic boundary condition [28]. One may find that the boundary condition is important for small systems. When the open boundary condition is chosen, one will find that the entanglement between every two spins varies as the site changes namely the
Fig. 1. Negativity in the mixed-spin system versus the parameter $\Delta$, and the system is at a low temperature $T = 0.02$. The cases of different system sizes $L = 4, 6, 8$ are considered. The inset is the first three energy levels of the 4-site case.

Fig. 2. Negativity in the spin-$1/2$ and spin-$1$ systems versus the parameter $\Delta$. The system size is $L = 6$, and the temperature is at $T = 0.02$.

entanglement oscillation occurs [29]. In our mixed-spin system, we chose the periodic boundary condition, then all the cells consisting of a spin-$1/2$ and a spin-$1$ are identical, and which is similar to the case of large-size system in the thermodynamic limit. Thus the periodic boundary condition is widely used in the research of spin-chain systems. In small systems considered by us, the energy structure has similar properties with the large-size systems. For example, at the isotropy point $\Delta = 1$, the degeneracy changes suddenly, which will also happen in the thermodynamic limit case. The entanglement can just capture the critical information. This is the reason that we choose the small-size system with periodic condition to present the critical properties of large-size system.

In Fig. 2, for comparison, we present the negativity of spin-$1/2$ and spin-$1$ systems versus parameter $\Delta$ as studied in Refs. [13,30]. We see that the negativity reaches its maximum at $\Delta = 1$, which is distinct from that in the case of mixed-spin system as shown in Fig. 1. When considering the energy level structure, one can find that there does not exist ground-state energy level crossing in the spin-$1/2$ and spin-$1$ systems at $\Delta = 1$. Therefore, we confirm that the special behavior of entanglement at the isotropic point can well reflect the different structure properties of $(1/2, 1)$ mixed-spin system from the uniform spin systems.

Our result in Fig. 1, shows that the pairwise entanglement reaches its extremum at the critical point where the system possesses SU(2) symmetry and undergoes quantum phase transition. When the system approaches the critical point, the quantum fluctuation induces the transition from a gapless phase ($-1 < \Delta < 1$) to a gapped phase ($\Delta > 1$). At the critical point $\Delta = 1$, the ground state has nonvanishing long-range correlation. And the entanglement manifests distinct features at the point where quantum phase transition undergoes. Since the entanglement represents the symmetry of the system and also the correlations between different sites [12]. Generally, at the critical point correlations develop on all length scales, thus the entanglement should correspond for these correlations and present at long length scales. Just the change of the entanglement structure indicate the system undergoing a quantum phase transition. The corresponding phenomenon is that the entanglement gives a extremum at the critical point. Otherwise, since the mixed-spin system possesses a maximal degeneracy at the critical point, the entanglement presents a drop instead of a maximum as in the uniform-spin system in Fig. 2. From the results one can find that the pairwise entanglement can not only indicate the critical point of the $(1/2, 1)$ mixed-spin system, but also exhibit the different fundamental structure of the mixed-spin system from the uniform spin system.
3. Purity and fidelity

3.1. Purity

It is well known that state entanglement and mixedness are properties central to quantum information theory. The relation between entanglement and mixedness have attracted much attention [2–6]. Let us introduce the definition of purity, which is used to measure the degree of mixedness of a state described by density operator $\rho$. The purity of the state $\rho$ is quantified as

$$P(\rho) = \text{Tr}[\rho^2].$$

(4)

For a pure state, we have $P = 1$, while for a maximally mixed state, i.e., for a total mixture $\rho = I/d$, the purity reaches its minimal value $P = 1/d$, where $d$ is the dimension of $\rho$.

For our $(1/2, 1)$ mixed-spin system, we calculate the purity for both the total system and the subsystems. First, considering the purity of a degenerate ground state of the total system, we can easily obtain the value of purity $P = 1/\alpha$, where $\alpha$ is the degeneracy of the ground states and in the $(1/2, 1)$ mixed-spin system $\alpha = 1 + L/2$. Especially, for small-size systems, such as $L = 4, 6, 8$, the purity of ground states reaches its minimum at the isotropic point with the values $P_{\text{min}} = 1/3, 1/4$ and $1/5$ respectively. Then the purity of the subsystem state $\rho_{1,2}$ is numerically studied, and the results are shown in Fig. 3. We see that the purity of the subsystem achieves the minimal value at the isotropic point. This implies that the purity of the subsystem can also exhibit the special property of the whole system.

In the quantum information theory, the entanglement and mixedness can be used to determine the frontier states, which possess the maximum amount of entanglement for a given degree of mixedness. These states may be useful in quantum information processing in the presence of noise [5]. The two concepts of entanglement and mixedness are closely related with each other [2–6]. For a general density matrix the purity (mixedness) of the state provides complementary information about the state. And the purity (mixedness) also preserves the fundamental information of the system such as the symmetry, the energy structure of the system and nonlocal correlations [4]. In our study, both the global purity and the partial purity to a reduced density display singularity at the critical point, and which is directly caused by the increscent degeneracy of the ground states at the SU(2) point. It is believed that the purity of states can indicate the critical point in some systems with quantum phase transition.

3.2. Fidelity

In this subsection, we will make use of the concept of the mixed state fidelity to investigate this mixed-spin system. Firstly, let us give the definition of the mixed state fidelity [31,32]

$$F(\rho_0, \rho_1) \equiv \text{Tr}\left(\sqrt{\rho_1^{1/2}\rho_0\rho_1^{1/2}}\right) = \sum_i \sqrt{\lambda_i}. $$

(5)

where the $\lambda_i$ is the eigenvalues of $\rho_1^{1/2}\rho_0\rho_1^{1/2}$. In our system, $\rho_0$ is the thermal state corresponding to the Hamiltonian $H_0$ in Eq. (1), and $\rho_1$ is easily obtained from $\rho_0$ by replacing $\Delta$ with $\Delta + \epsilon$. Here $\epsilon$ is a small perturbation parameter. To cancel the dependence of fidelity on the small perturbation $\epsilon$, the conception fidelity susceptibility [19,33] was introduced with the definition

$$\chi_F = \lim_{\epsilon \to 0} \frac{-2 \ln F}{\epsilon^2} = \lim_{\epsilon \to 0} \frac{2(1 - F)}{\epsilon^2}. $$

(6)
Fig. 4. UPPER: In the mixed-spin system, the fidelity susceptibility versus the parameter $\Delta$ at a low temperature $T = 0.02$. The cases of different system sizes $L = 4, 6, 8$ are considered. NETHER: In the uniform spin-1/2 system, the fidelity susceptibility versus $\Delta$, and different system sizes $L = 4, 6, 8$ are also considered.

Firstly, we numerically study the fidelity susceptibility of the whole system and show the results in the upper subfigure of Fig. 4. The fidelity susceptibility presents a peak at the isotropic point $\Delta = 1$, while beyond the vicinity of the isotropic point, $\chi_F$ gives zero values. This means that the system is sensitive to the perturbation only in the vicinity of the critical point. It can be easily understood as this, around the critical point, a small perturbation will induce two distinct ground states, and the states defining different phases are expected to be quite distinguishable, at the critical point the system is very susceptible to the perturbations. As the system size increases, the peak becomes steeper and narrow, and the position of the peak value is almost exactly at the critical point. This remarkable phenomenon of susceptibility reflects the critical point of the system, at which the crossing of ground-state energy levels happens and the degeneracy is changed.

For comparison, we plot the fidelity susceptibility of spin-1/2 system in the nether subfigure of Fig. 4. There is no peak appearing as in the mixed-spin system. With the increasing of system size, the susceptibility $\chi_F$ tends to give a minimum at the isotropic point, and oscillates as $\Delta$ varies. Moreover, the susceptibility is very weak, which means the ground state of this system is not susceptible to perturbation. This is also because the spin-1/2 system has no ground-state level crossing at the isotropic point [20]. From this point of view, the fidelity susceptibility can indicates the appearance of energy level crossing. In fact, lots of quantum critical phenomena emerge just at the point where energy level crossing occurs. Therefore, in the mixed-spin system, the fidelity susceptibility is an effective indicator of the quantum criticality.

We also consider the fidelity of the reduced density matrix $\rho_{1,2}$. The elements in the reduced density matrix contain the information of the whole system, thus we expect the fidelity of $\rho_{1,2}$ can also indicate the critical point. As shown in Fig. 5, the susceptibility of the reduced density matrix $\rho_{1,2}$ exhibits a sudden peak at the critical point. With the system size increasing, the position of the peak value tends to the point $\Delta = 1$. This phenomenon is nearly the same as that in the upper subfigure in Fig. 4 except that the susceptibility of $\rho_{1,2}$ is weaker, and the value is about one tenth of the whole system susceptibility. This is not surprising, since the reduced density only contains partial information of the overall system. Thus the fidelity susceptibility of subsystem can also indicate the critical point [34]. In many-body systems, it is usually difficult for us to study the whole system, thus it is a feasible and a practical way to consider the subsystem.

The fidelity used in this paper can distinguish the two states (pure or mixed) which have only slightly different values of the external parameter. It can be expected that if the two states belong to the same phase, the slightly different one between them will not be detected. However, when the system approaches the critical point, a small perturbation of the external parameter will make the two states come into two different phases, then the remarkable difference between the
In the mixed-spin system, the fidelity susceptibility of the reduced density $\rho_{1,2}$ versus the parameter $\Delta$ at a low temperature $T = 0.02$. The cases of different system sizes $L = 4, 6, 8$ are considered.

two states can be detected by the fidelity (fidelity susceptibility). In our results, we can see that both the fidelity susceptibility of the global system and the subsystem present singular behavior at the isotropy point, which indicates the critical point of the mixed-spin system. However, the ground state fidelity is not effective in the uniform spin system, which is because the quantum phase transition in the spin-$1/2$ XXZ system is induced by the excited energy level crossing and not by the ground energy level crossing [20]. And the different behaviors of the fidelity susceptibility also reflect the different fundamental structure of the mixed-spin system from the uniform spin system.

4. Conclusions

We investigate the ground-state entanglement, purity and fidelity in the $(1/2, 1)$ mixed-spin Heisenberg XXZ chain. A key step for our numerical calculation is to use the thermal state at low enough temperature to approximately represent the ground states of the system. This overcomes the subtle trouble induced by the energy degeneracy and gives a convenient form to characterize the ground states. First, we find that the entanglement, using the concept of negativity, presents a dip at the isotropic point, where the ground-state level crossing happens and the energy degeneracy changes suddenly. This phenomenon is quite different from the spin-$1/2$ uniform chain, whose entanglement exhibits a peak at the isotropic point. Then we show that the purity of the system achieves a minimum at the isotropic point as the ground states are maximally mixed. Finally, we also find that the fidelity susceptibility of the system shows a sharp peak at the isotropic point, while it does not appear in the spin-$1/2$ uniform system. From the study, we confirm that the three concepts of entanglement, purity and fidelity can indicate the quantum phase transition point of the $(1/2, 1)$ mixed-spin system. Otherwise, the behaviors of pairwise entanglement and fidelity susceptibility also reflect the different fundamental structure between $(1/2, 1)$ mixed-spin chain and spin-$1/2$ chain. In addition, it should be pointed out that though our calculations are restricted to the $(1/2, 1)$ mixed-spin system, the method in this paper is also applicable to other systems with quantum criticalities caused by ground-state level crossing, especially to the systems with continuously degenerate ground states.

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