Entanglement, quantum phase transition, and scaling in the *XXZ* chain

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Motivated by recent development in quantum entanglement, we study relations among concurrence C, $SU_q(2)$ algebra, quantum phase transition and correlation length at the zero temperature for the XXZ chain. We find that at the SU(2) point, the ground state possesses the maximum concurrence. When the anisotropic parameter Δ is deformed, however, its value decreases. Its dependence on Δ scales as $C=C_0-C_1(\Delta-1)^2$ in the XY metallic phase and near the critical point (i.e., $1<\Delta<1.3$) of the Ising-like insulating phase. We also study the dependence of C on the correlation length ξ, and show that it satisfies $C=C_0-1/2\xi$ near the critical point. For different sizes of the system, we show that there exists a universal scaling function of C with respect to the correlation length ξ.

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Quantum entanglement, as one of the most intriguing feature of quantum theory, has been a subject of much study in recent years, mostly because its nonlocal connotation [1] is regarded as a valuable resource in quantum-communication and Quantum-information processing [2,3]. For example, an entangled state, such as a singlet state $1/\sqrt{2}(|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle)$, can be used for the realization of teleportation [4]. On the other hand, as with other resources, such as free energy and information, one would like to know how it can be quantified and controlled. For the first problem, all of efforts have been devoted to develop a quantitative theory of entanglement, including entanglement of formation [5–8], which is regarded as its basic measure. For the second problem, many authors [9–17] tried to build a bridge between quantum entanglement and physical models by investigating their entanglement in both the ground state [9,16] and thermal state [14,15].

Very recently, the intriguing issue of the relation between entanglement and quantum phase transition has been addressed [17,18]. For a spin-1/2 ferromagnetic chain, Osterloh *et al.*, reported that the entanglement shows scaling behavior in the vicinity of quantum phase transition point [19] as induced by a transverse magnetic field. Vidal *et al.* tried to establish a connection between quantum-information and condensed-matter theory by studying the behavior of critical entanglement in spin systems. So it is believed that the entanglement of the ground state, like the conductivity in the Mott-insulator transition [20] and quantum Hall effect, and magnetization in the external-field-induced phase transition, also plays a crucial role in the understanding of quantum phase transition. On the other hand, group theory as well as symmetry of the system are parts of the foundation of quantum mechanics [21,22], the knowledge of its presence often makes it easy to understand the physics. Thus, the study of entanglement at the ground state and its relation to the group theory will not only have a contribution to experimental realization, but also enrich our physical intuition of quantum theory.

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The main focus of the present paper is to study the properties of ground state concurrence of an antiferromagnetic XXZ chain. We show that the competition between quantum fluctuation and ordering will lead to maximum value of concurrence at the isotropic point. This observation could also be clarified from the point of view of q-deformation theory. The concurrence's dependence on anisotropic parameter Δ is presented both numerically and analytically. The relation of the concurrence to the correlation length ξ in the Ising-like insulating phase as well as the scaling behavior around the critical point $\Delta=1$ where the metal-insulator quantum phase transition occurs are also discussed. Thus, our result not only manifest interesting physical phenomenon, but also establish nontrivial connection between the quantities in quantum-information theory and critical phenomenon, correlation length in condensed-matter physics and quantum group theory [22].

The Hamiltonian of the XXZ chain with periodic boundary conditions reads

$$H(\Delta)=\sum_{l}^{N}\left[\sigma_l^x\sigma_{l+1}^x+\sigma_l^y\sigma_{l+1}^y+\Delta\sigma_l^z\sigma_{l+1}^z\right],$$

$$\sigma_{N+1}=\sigma_1, \tag{1}$$

where N is the number of sites, $\sigma^\alpha(\alpha=x,y,z)$ are Pauli matrices, and Δ is a dimensionless parameter characterizing anisotropic interaction. The Hamiltonian is invariant under translation, therefore, the entanglement between arbitrary two neighbor sites is a uniform function of site index. At $\Delta=1$, Eq. (1) has SU(2) symmetry. While $\Delta\neq1$, it becomes q-deformed SU(2) algebra with $\Delta=(q+q^{-1})/2$. Together with the Z^2 symmetry, we can have $[H,S^z]=0$, which result in that the reduced density matrix $\rho_{l(l+1)}$ of two neighbor sites is of the form [9]

$$\rho_{l(l+1)}=\begin{pmatrix} u^+ & 0 & 0 & 0 \\ 0 & w_1 & z & 0 \\ 0 & z^* & w_2 & 0 \\ 0 & 0 & 0 & u^- \end{pmatrix} \tag{2}$$

in the standard basis $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$. Since the energy of a single pair in the system is $E/N=\mathrm{tr}[\rho_{l(l+1)}H_l]$, where H_l is the part of the Hamiltonian between site l and $l+1$, due to the translational invariance. Considering the definition of entanglement, we can easily find that the concurrence of XXZ chain can be calculated as [13,23]

$$C=\tfrac{1}{2}\max(0,|E/N-\Delta G^{zz}_{l(l+1)}|-G^{zz}_{l(l+1)}-1), \qquad (3)$$

where $G^{zz}_{l(l+1)}$ is the correlation function. So we not only need to know the energy of the system, but also the behavior of correlation function.

It is well known that the present model can be exactly solved by quantum inverse method [24,25], and its energy spectra are determined by a set of spin rapidities $\lambda_1,\lambda_2,\ldots,\lambda_M$, which describe the kinetic behavior of a state with M down spins. They are the solution of Bethe-ansatz equation

$$\left(\frac{\sinh\gamma(\lambda_j+i)}{\sinh\gamma(\lambda_j-i)}\right)^N=\prod_{l\neq j}^{M}\frac{\sinh\gamma(\lambda_j-\lambda_l+2i)}{\sinh\gamma(\lambda_j-\lambda_l-2i)}, \qquad (4)$$

where the parameter γ arises from the anisotropic scale Δ, i.e., $\Delta=\cos 2\gamma$. The regime $0<\Delta<1$ is characterized by real positive γ while the regime $1<\Delta$ by pure imaginary γ with positive imaginary part. When $\gamma\to 0$, the above secular equations reduce to the well known one for isotropic Heisenberg model.

Taking the logarithm of the above equation, we can have a set of transcendental equations for $\{\lambda_j\}$, in which the energy level is determined by a set of quantum number $\{I_j\}$. For the ground state, $\{I_j\}$ are consecutive integer or half-odd-integer centering around zero and $M=N/2$. Then the ground-state energy of the system can be calculated either by solving the Bethe-ansatz equations numerically for finite-size system or by solving integral equation of density function of λ in the thermodynamic limit. Once the Δ dependent eigenenergy $E(\Delta)$ is obtained, the correlation function is simply the first derivative of $E(\Delta)/N$ with respect to Δ.

For the XXZ model, there exist two different phases at the ground state, i.e., metallic phase, $0<\Delta\leqslant 1$, and insulating phase, $\Delta>1$, which is resulted from that the former is gapless while the latter is gapful. The critical point of quantum phase transition locates at the isotropic point $\Delta=1$ at which the concurrence is just a simple function of ground-state energy per sites, i.e., 0.386. If we regard σ^z as a 'coordinate', then the first two terms in Eq. (1) represent the ''kinetic energy'' causing the quantum fluctuations of σ^z, and the last term represents the ''potential energy'' that causes the ordering of σ^z. In the Ising limit $\Delta\to\infty$, the ground state has the Néel long-range order, which results in the concurrence being zero. When Δ becomes smaller but still larger than 1, the quantum fluctuation plays a more and more important role, then the Néel state is no longer an eigenstate of the Hamiltonian. This fluctuation between two neighboring sites enhances the value of off-diagonal term z in their reduced density matrix $\rho_{l(l+1)}$, then the entanglement becomes larger and larger. On the other hand, at the free particle (XX) limit where $\Delta=0$, the spin-flip term dominates the system completely and all spins flip freely on lattice sites. For a certain site j, the probability of spin up and down is the same, regardless of the spin state of its neighbor. Thus, the state $|\uparrow\uparrow\rangle$ will not lower the energy, but share the same probability with $|\downarrow\uparrow\rangle$ or $|\uparrow\downarrow\rangle$. This phenomenon will result in a relatively large u^+ or u^- in the reduced density matrix of two neighbor sites, as well as a relative smaller C. On the contrary, once the anisotropic interaction $1>\Delta>0$ is turned on, the value of u^+ and u^- is lowered. So the concurrence is enhanced. Hence the competition of quantum fluctuation and ordering must result in a maximum concurrence at a certain point. Comparing with the origin of metal-insulator transition in the present model, which also arises from the competition of fluctuation and ordering, it is natural to infer that the point we want here is just the isotropic point, i.e., $\Delta=1$, as illustrated in Fig. 1. This case is very similar to the formation of Kondo effect, in which the competition between spin singlet formation and thermal conductivity leads to a minimum conductivity at the Kondo temperature. The idea can also be applied to the entanglement of arbitrary two sites, such as the concurrence C_{lm} between site l and m. Only when the competition between their interaction and fluctuation reaches a counterbalance, the concurrence C_{lm} reaches its maximum.

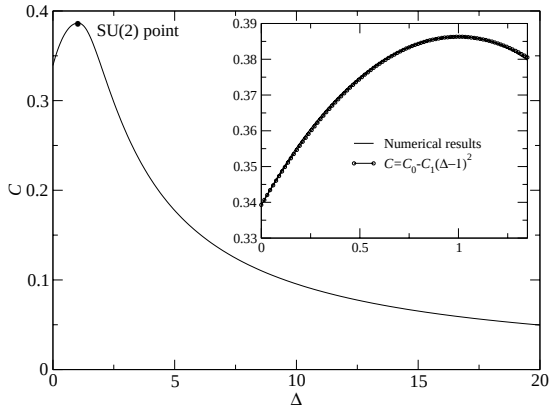

FIG. 1. Representation of concurrence C as a function of Δ, obtained by solving three sets of Bethe-ansatz equations of $N=1280$ sites system numerically. It is clear that the concurrence reach is maximum at the critical point $\Delta=1$.

From the quantum group theory point of view, at $\Delta=1$ point, the ground state is SU(2) singlet in which the two neighboring sites try to form antisymmetric pair, as $(|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle)/\sqrt{2}$. In the q-deformed region, Hamiltonian (1) can be rewritten in terms of Temperly Lieb operators

$$H=N\Delta+2\sum_{j}^{N}T_{j,j+1}, \qquad (5)$$

where $T_{j,j+1}=\{-q^{-1},1;1,-q\}$ in the basis $|\uparrow\downarrow\rangle,|\downarrow\uparrow\rangle$. Define q-deformed antisymmetric state $|\phi_q\rangle=(|\uparrow\downarrow\rangle-q|\downarrow\uparrow\rangle)/\sqrt{1+q^2}$, then the operator $T_{j,j+1}$ can be expressed as $T_{j,j+1}=-(\Delta/2)|\phi_q\rangle\langle\phi_q|$. If $\Delta>1$, the lowest-energy state favors the formation of q-deformed antisymmetric state between two neighboring sites [26], unlike the case of $\Delta=1$ where it favors antisymmetric state, which obviously

leads to the decrease of concurrence between two neighboring sites. When the deformation parameter q becomes very large, it tends to the Néel state. On the other hand, the $|\phi_q\rangle$ breaks the local translational invariance, from the point of view of spinless fermions model, the formation of $|\phi_q\rangle$ develops charge-density state at the ground state, which is gapped and low symmetric.

We show the concurrence as a function of Δ in Fig. 1, which is obtained by solving both the Bethe-ansatz equations for 1280 sites system numerically, and the integral equation for infinite length system (We obtained the same result). As we expected, the ground state at the isotropic point possessed the maximum concurrence. Thus, symmetry of the Hamiltonian plays a central role in determining the concurrence of its ground state. And the trend of curve can be easily understood based on the above argument. On the other hand, a challenging and nontrial problem is to quantify the concurrence around the critical point. In the XY metallic phase and near the critical point (i.e., $1<\Delta<1.3$) of the Ising-like insulating phase, it is amazing that C can be described by

$$C=C_0-C_1(\Delta-1)^2 \tag{6}$$

very well, where

$$C_0=2\ln 2-1\simeq 0.386,$$

$$C_1=2\ln 2-\frac{1}{2}-\frac{2}{\pi}-\frac{2}{\pi^2}\simeq 0.047, \tag{7}$$

as illustrated in the inset of Fig. 1. Hence around $\Delta=1$, the critical exponents of the anisotropic term is 2. As we know, the present model can be transformed into spinless fermions model by Jordan-Wigner transformation. For the free particle case, it is easy to obtain that the ground-state energy and the correlation function G^{zz} are $4/\pi$, and $4/\pi^2$, respectively. In the large Δ limit, we find the concurrence scales like $C\propto 1/\Delta$. One can also express C in terms of deformation factor q via the relation $q=\Delta\pm\sqrt{\Delta^2-1}$. It has the form

$$C=C_0-\frac{C_1}{4}(q^{1/2}-q^{-1/2})^4 \tag{8}$$

around the critical point. In XY metallic phase, if we define $q=e^{i\phi}$, it becomes

$$C=C_0-4C_1\sin^4\frac{\phi}{2}. \tag{9}$$

Now we study the scaling behavior in the Ising-like insulating phase by considering the correlation length. Though the scaling study of metal-insulator transition based on the analysis of spin stiffness has been proposed recently [27], and though everyone believe there must exist some relation between correlation and entanglement, the scaling of concurrence, and its dependence on the correlation length still remains an open and interesting problem. By analyzing the finite chain system, one can obtain the correlation length as a function of Δ in an easy way [27,28]. It has the form

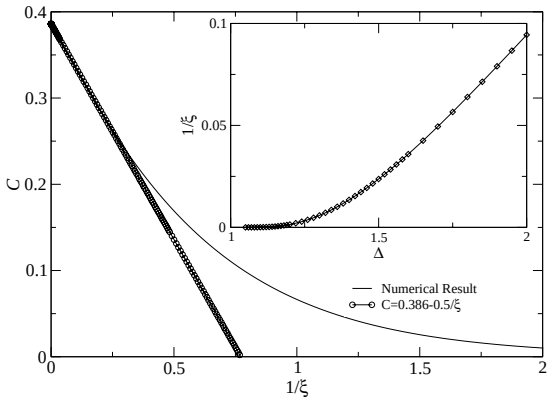

FIG. 2. Representation of concurrence C as a function of $1/\xi$. Here ξ is in unit of lattice constant.

$$1/\xi=\gamma+\sum_{n=1}^{\infty}\frac{(-1)^n}{n}\tanh(2n\gamma), \tag{10}$$

In the $\Delta\to 1$ limit, it has a good approximation, as $1/\xi\propto(\Delta-1)^2$. Clearly, the correlation length is independent of system size, its behavior is shown in the inset of Fig. 2. The dependence of C on ξ is represented in Fig. 2, in which the solid line is obtained by solving Bethe-ansatz equations for 1280 sites system numerically. For the value of ξ bigger than 4, i.e., $1/\xi<0.25$, there exists a simple relation between C and ξ, which scales

$$C=C_0-\frac{1}{2\xi}. \tag{11}$$

The above equation implies that the concurrence does not have a long-range effect, in another way, we can say that a small system, such as $N=20$, can well describe the behavior of concurrence of large system, as illustrated in Fig. 3. Compared with the scaling of spin stiffness [27], the present one is more perfect, that is, the concurrence is almost independent of the system size when $L>10$. So we can conclude that for finite-size system, there exists a scaling function,

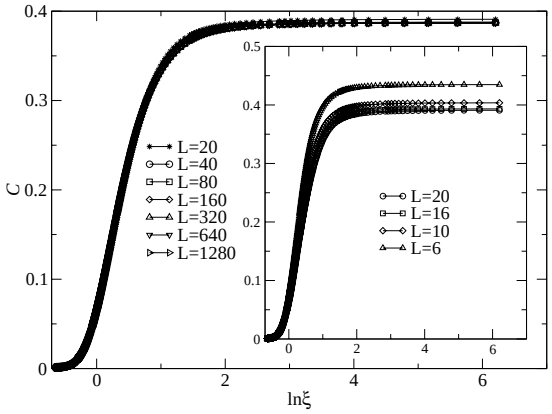

FIG. 3. Representation of concurrence C as a function of ξ for different system sizes.

which is independent of L and scales like Eq. (11) in large ξ limit. Only when $L<10$, the finite-size effect becomes very clear (See the inset of Fig. 3). Moreover, for small system, concurrence in even number sites and odd ones is different. The former is usually larger than the latter due to the frustration effect happens in odd sites system with periodic boundary condition. For example, for three sites system, the two singlet formations between sites 1, 2 and between sites 2, 3 break singlet formation of sites 3, 1. When L becomes large, these effects can be neglected and the concurrence in two cases are the same.

In summary, we have investigated the ground state concurrence of the XXZ chain. We pointed out that the competition between quantum fluctuation and Néel ordering will lead to a maximum value of concurrence at the isotropic Heisenberg point. Based on the Bethe-ansatz solution, we exactly obtained the dependence of C on the parameter Δ in a wide range around the critical point and the numerical result in the whole range. We established the relation between the concurrence and deformation factor q of quantum group in the Ising-like insulating phase. It is now clear that q-deformed permutation generator favors the formation of a deformed ground state, which has a relatively smaller concurrence. Moreover, the relation between the concurrence and the correlation length was studied both numerically and analytically. We found that there exists a universal scaling behavior for finite- (not small) size system and it satisfies a simple relation $C \propto 1/2\xi$ in the region close to the critical point.

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