Entanglement, quantum phase transition and scaling in XXZ chain

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Motivated by recent development in quantum entanglement, we study the 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 $\Delta$ is deformed, its value decreases. Its dependence on $\Delta$ 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 $\xi$, and show that it satisfies $C = C_0 - 1/2\xi^2$ near the critical point. For different size of the system, we show that there exists a universal scaling function of $C$ with respect to the correlation length $\xi$.

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Quantum entanglement, as one of the most intriguing features 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 information processing$^2,3$. For example, an entangled state, such as a singlet state $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$, 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, much efforts have been devoted to develop a quantitative theory of entanglement, including entanglement of formation$^5,6,7,8$, which is regarded as its basic measure. For the second problem, many authors$^9,10,11,12,13,14,15,16,17$ tried to build a bridge between quantum entanglement and physical models by investigating their entanglement in both the ground state$^9,10$ and thermal state$^{14,15}$.

Very recently, the intriguing issue of the relation between entanglement and quantum phase transition has been addressed$^{14,15}$. 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, is also plays a crucial role to 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 enrichs our physical intuition of quantum theory.

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 view of $q$-deformation theory. The concurrence’s dependence on anisotropic parameter $\Delta$ is presented both numerically and analytically. The relation of the concurrence to the correlation length $\xi$ 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 non-trivial 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

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

$$\sigma_{N+1} = \sigma_1,$$ (1)

where $N$ is the number of sites, $\sigma^\alpha$ ($\alpha = x, y, z$) are Pauli matrices, and $\Delta$ 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 $\Delta \neq 1$, 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 $\rho_{l(t+1)}$ of two neighbor sites is of the form

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

(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 $E/N = tr[\rho_{l(t+1)}H_l]$, where $H_l$ is the part of Hamiltonian between site $l$ and $l+1$, due to the translational invariance. Considering the definition of entanglement, we can easily obtain that the concurrence of XXZ chain can be written as

$$
C = \frac{1}{2} \max \{0, |E/N - \Delta G_{l(l+1)}^{zz} - G_{l(l+1)}^{zz} - 1\}.
$$

(3)

where $G_{l(l+1)}^{zz}$ 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,

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

$$
\frac{\sinh \gamma (\lambda_j + i)}{(\sinh \gamma (\lambda_j - i)} = \prod_{l \neq j} \frac{\sinh \gamma (\lambda_j - \lambda_l + 2i)}{\sinh \gamma (\lambda_j - \lambda_l - 2i)}
$$

where the parameter $\gamma$ arises from the anisotropic scale $\Delta$, i.e., $\Delta = \cos 2\gamma$. The regime $0 < \Delta < 1$ is characterized by real positive $\gamma$ while the regime $1 < \Delta$ by pure imaginary $\gamma$ 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 of $\lambda$ in the thermodynamic limit. Once the $\Delta$ dependent eigenenergy $E(\Delta)$ is obtained, the correlation function is simply the first derivative of $E(\Delta)/N$ with respect to $\Delta$.

For the XXZ model, there exist two different phases at the ground state, i.e., metallic phase: $0 < \Delta \leq 1$ and insulating phase: $\Delta > 1$, which is resulted from that the former is gapless while the later 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 $\sigma^z$ as a ‘coordinate’, then the first two terms in Eq. represent the ‘kinetic’ energy causing the quantum fluctuations of $\sigma^z$, and the last term represents the ‘potential energy’ that causes the ordering of $\sigma^z$. In the Ising limit $\Delta \to \infty$, the ground state has the Néel long-range-order, which results in that the concurrence is zero. When $\Delta$ becomes smaller but still large than 1, the quantum fluctuation plays 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 $\rho_{l(t+1)}$, 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 the spin state of its neighbor. Thus the state $|\uparrow\uparrow\rangle$ will not lower the energy, but share the same probability with $|\downarrow\downarrow\rangle$ or $|\downarrow\uparrow\rangle$. 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 results in a maximum concurrence at a certain point. Comparing with the origin of metal-insulator transition in the present model, which also arise 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 the Fig.

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.

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, the Hamiltonian

can be rewritten in terms of Temperly-Lieb operators

$$
H = N \Delta + 2 \sum_{j} T_{j,j+1},
$$

(5)

where $T_{j,j+1} = \{-q^{-1}, 1, -q\}$ in the basis $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$. 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 $T_{j,j+1} = -i\frac{d}{d\phi_q}$. If $\Delta > 1$, the lowest energy state favor the formation of $q$-deformed antisymmetric state between two neighboring sites, 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 view of spinless fermions model, the
formation of $|\phi_q\rangle$ develops charge-density-state (CDW) at the ground state, which is gapped and low symmetric.

We show the concurrence as a function of $\Delta$ 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 expect, the ground state at the isotropic point possesses 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 challenge and non-trial 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

$$C = C_0 - C_1(\Delta - 1)^2,$$

very well, where

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

$$C_1 = 2\ln 2 - \frac{1}{2} - \frac{2}{\pi} \approx 0.047,$$

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 $\Delta$ 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 $q = \Delta + \sqrt{\Delta^2 - 1}$. It has the form

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

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

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

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 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 $\Delta$ in an easy way [27, 28]. It has the form

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

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. 1. The dependence of $C$ on $\xi$ 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 $\xi$ bigger than 4, i.e. $1/\xi < 0.25$, there exist a simple relation between $C$ and $\xi$, which scales

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

The above equation imply that the concurrence of does not have a long-range effect, in another way, we can say that a smallish 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 exist a scaling function, which is independent of $L$ and scales like Eq. (11) in large $\xi$ 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 one is different. The former is usually larger than the later due to the frustration effect happens in odd sites system with periodic boundary condition. For example, for 3 sites system, the two singlet formations between sites 1, 2 and between sites 2, 3 breaks singlet formation of sites 3, 1. When \( L \) becomes large, this effects can be neglected and the concurrence in two case is 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 \( \Delta \) in a wide range around the critical point, and obtained 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 critic point.

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