The ground state entanglement in the XXZ model

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In this paper, we investigate spin entanglement in the XXZ model defined on a \( d \)-dimensional bipartite lattice. The concurrence, a measure of the entanglement between two spins, is analyzed. We prove rigorously that the ground state concurrence reaches maximum at the isotropic point. For dimensionality \( d \geq 2 \), the concurrence develops a cusp at the isotropic point and we attribute it to the existence of magnetic long-range order.

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Entanglement, as the exhibition of pure quantum correlations between separate systems, has become one of the trademarks of the quantum mechanics for its non-local connotations\textsuperscript{1,2}. Recently, many physicists have made great efforts to understand the quantum entanglement in the ground states of some many-body spin models\textsuperscript{3-11}. One expects that a thorough investigation on the entanglement in these systems will provide new insight into the quantum phase transition in many-body spin models, such as the spin ladder model and, in particular, the XXZ model in higher dimensions\textsuperscript{12}. It is well known that, as far as the above-mentioned properties are concerned, the ground states of these models are akin to the antiferromagnetic XXZ chain.

This paper contains two parts. In the first part, based on some well-known facts about the antiferromagnetic spin models, we prove rigorously that, when the antiferromagnetic XXZ model is defined on a \( d \)-dimensional finite bipartite lattice, the concurrence between two spins located on a pair of nearest-neighbor sites is an analytical function of the anisotropic parameter and takes on its maximum at the Heisenberg isotropic point. Then, in the second part of this paper, justified by the existence of magnetic long-range order (LRO) in the XXZ model, we use the spin-wave theory to show that a cusp-like behavior of the concurrence develops in the thermodynamic limit when the dimensionality of the lattice \( d \geq 2 \).

To begin with, we first introduce several notations. On a finite \( d \)-dimensional simple cubic lattice \( \Lambda \) with \( |N_\Lambda| = L^d \) sites, the Hamiltonian of the antiferromagnetic XXZ model is

\[ \hat{H}_{\text{XXZ}} = \sum_{\langle ij \rangle} \left( \hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + \Delta \hat{S}_i^z \hat{S}_j^z \right), \]  (1)

where \( \hat{S}_i^x \) and \( \hat{S}_i^y \) are spin-1/2 operators at site \( i \) and \( \Delta = J_z/J_x \) is a dimensionless parameter characterizing the anisotropy of the model. The sum in the Hamiltonian is over all pairs of nearest-neighbor sites \( i \) and \( j \). Obviously, this Hamiltonian commutes with the total spin-1/2 operator \( \hat{S}^z_{\text{total}} = \sum_i \hat{S}_i^z \). Thus, each eigenstate of the Hamiltonian is also an eigenstate of \( \hat{S}^z_{\text{total}} \). Consequently, the Hilbert space of the system can be decomposed into numerous subspaces \( V(M) \). In each subspace, the spin number \( \hat{S}^z_{\text{total}} = M \) is specified. It is well known that, on a finite simple cubic lattice \( \Lambda \), the ground state of the XXZ model is nondegenerate in any admissible subspace \( V(M) \)\textsuperscript{13,14}. In particular, its global ground state \( \Psi_0(\Lambda, \Delta) \), which coincides with the ground state of the model in the subspace \( V(M = 0) \)\textsuperscript{15,16}, is also nondegenerate. Therefore, all the physical quantities, such as the ground state energy \( E_0(\Lambda, \Delta) \) and the spin correlation function \( \langle \hat{S}_i^z \hat{S}_j^z \rangle \) are analytical functions of the parameter \( \Delta \), as long as the lattice is finite.

The conservation of \( \hat{S}^z_{\text{total}} \) implies also that, with respect to the standard basis vectors \( |\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\downarrow\rangle \) and
As a result, the concurrence of the two spins is
\[ C_{ij} = 2 \max \left( |G^{zx}_{ij} + G^{yy}_{ij}| - G^{zz}_{ij} - \frac{1}{4}, 0 \right). \] (3)

By the variational principle, one can show that all the spin correlations functions \( G^{m\alpha}_{ij} \) are negative. Thus, one has
\[ C_{ij} = \left( -G^{zx}_{ij} - G^{yy}_{ij} - \frac{1}{4} + G^{zz}_{ij} \right) \]
\[ = \left( -e_{ij}^{0}(\Lambda, \Delta) - \frac{1}{4} + (\Delta - 1)G^{zz}_{ij} \right), \] (4)
where \( e_{ij}^{0}(\Lambda, \Delta) = E_{0}(\Lambda, \Delta)/N_{B} \) \( (N_{B} \) is the number of bonds in the lattice) is the ground state energy per bond. Furthermore, since all quantities in \( C_{ij} \) are analytical functions of the parameter \( \Delta \), we are allowed to take derivatives of it with respect to \( \Delta \). In particular, after taking the first order derivative of \( C_{ij} \), we obtain
\[ \frac{\partial C_{ij}}{\partial \Delta} = 2 \left( -\frac{\partial e_{ij}^{0}(\Lambda, \Delta)}{\partial \Delta} + G^{zz}_{ij} + (\Delta - 1) \frac{\partial G^{zz}_{ij}}{\partial \Delta} \right). \] (5)

Again, due to the nondegeneracy of the global ground state \( \Psi_0(\Lambda, \Delta) \) of the XXZ model on a finite lattice, we can use the Hellmann-Feynman theorem to calculate the derivative \( \frac{\partial e_{ij}^{0}(\Lambda, \Delta)}{\partial \Delta} \), which equals to \( G^{zz}_{ij} \). Therefore, we finally obtain
\[ \frac{\partial C_{ij}}{\partial \Delta} = 2 (\Delta - 1) \frac{\partial G^{zz}_{ij}}{\partial \Delta} \]
\[ = 2 (\Delta - 1) \frac{\partial^2 e_{ij}^{0}(\Lambda, \Delta)}{\partial \Delta^2}. \] (6)

Immediately, one sees that \( \Delta = 1 \) is an extreme point of the concurrence.

Next, we show that \( \Delta = 1 \) is actually a maximal point of \( C_{ij} \) and the concurrence does not have other extreme point. In fact, both the statements are the corollaries of concavity of the ground state energy \( E_{0}(\Lambda, \Delta) \) of the Hamiltonian \( \hat{H}_{XXZ} \) with respect to the anisotropic parameter \( \Delta \). By the variational principle, we know that, for any two parameters \( \Delta_{1} \) and \( \Delta_{2} \), the following inequality
\[ E_{0}(\Lambda, \lambda \Delta_{1} + (1-\lambda)\Delta_{2}) \geq \lambda E_{0}(\Lambda, \Delta_{1}) + (1-\lambda)E_{0}(\Lambda, \Delta_{2}), \] (7)
where \( 0 \leq \lambda \leq 1 \), holds true for the ground state energy \( E_{0}(\Lambda, \Delta) \). In particular, when \( E_{0}(\Lambda, \Delta) \) is differentiable with respect to \( \Delta \), inequality (7) is equivalent to
\[ \frac{\partial^2 E_{0}(\Lambda, \Delta)}{\partial \Delta^2} \leq 0. \] (8)

Consequently, we have also \( \frac{\partial^2 C_{ij}^{0}(\Lambda, \Delta)}{\partial \Delta^2} \leq 0 \). Now, let us take derivative of Eq. (6) again with respect to \( \Delta \). It yields
\[ \frac{\partial^2 C_{ij}}{\partial \Delta^2} \bigg|_{\Delta = 1} = 2 \frac{\partial^2 e_{ij}^{0}(\Lambda, \Delta)}{\partial \Delta^2} \bigg|_{\Delta = 1} \leq 0. \] (9)

Therefore, \( \Delta = 1 \) is indeed a maximal point of the concurrence.

Finally, we prove that \( \Delta = 1 \) is the unique extreme point of the concurrence \( C_{ij} \). For that purpose, we notice that inequality (8) is actually strict. In other words, the equal sign in it can be ignored. This can be easily understood by observing the following fact: As \( \Delta \) increases from \(-\infty \) to \( \infty \), quantity \( \langle \hat{S}_i^z \hat{S}_j^z \rangle = \partial e_{ij}^{0}(\Lambda, \Delta)/\partial \Delta \) becomes more and more negative. Consequently, the product on the right-hand side of Eq. (6) cannot be zero at any point except \( \Delta = 1 \). That completes our discussion on the general behavior of the concurrence \( C_{ij} \) for the antiferromagnetic XXZ model on a finite d-dimensional simple cubic lattice. In addition, we point out that the above proof can be easily extended to other cases, such as the spin ladder model at \( J_z = 0 \).

In the following, we shall discuss the behavior of the concurrence in the thermodynamic limit. In Ref. [18], by using the Bethe ansatz solution of the one-dimensional XXZ chain, we obtained the explicit expression of the concurrence near the isotropic point
\[ C_{i,i+1} = C_0 - C_1 (\Delta - 1)^2, \] (10)
where \( C_0 \) and \( C_1 \) are two real constants. Therefore, the concurrence of the 1D XXZ chain is a differentiable function of \( \Delta \) in the thermodynamic limit. However, things are quite different in higher dimensions. For the XXZ model in higher dimensions, there exists no exact solution. One either uses approximate analytical approach such as the spin-wave theory or numerical approach such as exact diagonalization studies of finite lattice. To obtain results in the thermodynamic limit, finite size scaling analysis must be performed. By using the stochastic series expansion quantum Monte Carlo method for lattices up to \( 16 \times 16 \), Sandvik [21] did an extensive study on the two-dimensional \( S=1/2 \) antiferromagnetic Heisenberg model. The finite size results for various ground state quantities were extrapolated to the thermodynamic limit using fits to polynomials in \( 1/L \), constrained by scaling forms previously obtained from renormalization-group calculations for the nonlinear sigma model and chiral perturbation theory. He demonstrated that the results were fully consistent with the predicted leading finite size corrections. With the same scaling forms, Lin,
Flynn, and Betts studied the XXZ model on square lattices and obtained various quantities as functions of anisotropic parameter $\Delta$ for the infinite system. Two conclusions from pervious works are relevant to the present study: (i) results obtained from the spin-wave theory are qualitatively correct and quite accurate, usually within 3 percent as compared with exact solution on finite lattices; (ii) derivatives of the ground state energy with respect to the anisotropic parameter $\Delta$ are not continuous at the Heisenberg point $\Delta = 1$, for example, see Figure 3 in Ref. [21]. This conclusion is consistent with the belief that there exists antiferromagnetic long-range order (LRO) in the d-dimensional XXZ model for $d \geq 2$. In fact, the existence of the LRO for $d \geq 3$ was rigorous proved, while for $d = 2$ most numerical studies support it. Based on these conclusions, we apply the spin-wave theory to calculate the concurrence $C_{ij}$ of the XXZ model. We also use exact diagonalization results as complementary. As shown in the following, the symmetry breaking in the thermodynamic limit, which is absent in the one-dimensional case, causes the singular behavior of the concurrence at the quantum phase transition point.

Following the standard procedure, the XXZ Hamiltonian is mapped into a boson model via the Holstein-Primakoff (HP) transformation

$$
\hat{S}_i^+ = \sqrt{2S}(1 - \hat{n}_i/2S)^{1/2}\hat{a}_i \simeq \sqrt{2S}(1 - \hat{n}_i/4S)\hat{a}_i,
$$
$$
\hat{S}_i^- = \sqrt{2S}\hat{a}_i^\dagger(1 - \hat{n}_i/2S)^{1/2} \simeq \sqrt{2S}\hat{a}_i^\dagger(1 - \hat{n}_i/4S),
$$
$$
\hat{S}_i^z = S - \hat{a}_i^\dagger\hat{a}_i,
$$

(11)

where $\hat{a}_i$ and $\hat{a}_i^\dagger$ are boson creation and annihilation operators at site $i$ for the spin deviation. In the region $\Delta > 1$, the antiferromagnetic ordering is in the spin-$z$ direction. Consequently, we have

$$
\hat{H}_{XXZ}/\Delta \simeq \sum_{ij} \left[ -S^2 + S \left( \hat{a}_i^\dagger\hat{a}_i + \hat{a}_j^\dagger\hat{a}_j \right) \right] + xS \left( \hat{a}_i\hat{a}_j + \hat{a}_i^\dagger\hat{a}_j^\dagger \right),
$$

(12)

where $x = 1/\Delta$. Using Fourier transform, we rewrite the Hamiltonian as

$$
\hat{H}_{XXZ}/\Delta = -\frac{z}{2}NS^2 + zS\sum_{\mathbf{k}} \hat{H}(\mathbf{k}),
$$

(13)

where $z$ is the coordination number of the lattice and

$$
\hat{H}(\mathbf{k}) = \hat{a}_k^\dagger\hat{a}_k + \frac{x\gamma_k}{2} \left( \hat{a}_k\hat{a}_{-\mathbf{k}} + \hat{a}_k^\dagger\hat{a}_{-\mathbf{k}}^\dagger \right),
$$

(14)

with $\gamma_k = \frac{2}{z}\sum_{m=1}^{z} \cos k_m$. By applying the Bogoliubov transformation

$$
\hat{a}_k = u_k\hat{c}_k - v_k\hat{c}_k^\dagger,
$$
$$
\hat{a}_k^\dagger = -v_k\hat{c}_k + u_k\hat{c}_k^\dagger,
$$

(15)

we diagonalize $\hat{H}(\mathbf{k})$ and obtain

$$
\hat{H}(\mathbf{k}) = v_k^2 - x\gamma_k u_k v_k + \left( u_k^2 + v_k^2 - 2xu_k v_k \gamma_k \right) \hat{c}_k^\dagger\hat{c}_k,
$$

(16)

where the $u_k$ and $v_k$ satisfy the following constraint conditions

$$
u_k^2 - v_k^2 = 1, \quad \frac{x\gamma_k}{2}(u_k^2 + v_k^2) - u_k v_k = 0.
$$

(17)

Finally, the ground state energy of the model in the region of $\Delta > 1$ can be written as

$$
E_0(\Delta > 1) = -\frac{z}{2}NS^2 + \frac{zS}{2}\sum_{\mathbf{k}} \left( \sqrt{1 - x^2\gamma_k^2} - 1 \right).
$$

(18)

By similar approach, we can also obtain the ground state energy of the XXZ model in the parameter region of $0 < \Delta < 1$. In this case, the system has antiferromagnetic order in the XY plane in the thermodynamic limit. As a result, the diagonalized Hamiltonian has the following form

$$
\hat{H}(\mathbf{k}) = (1 + y\gamma_k) v_k^2 - x\gamma_k u_k v_k + \left[ (1 + y\gamma_k)(u_k^2 + v_k^2) - 2xu_k v_k \gamma_k \right] \hat{c}_k^\dagger\hat{c}_k.
$$

(19)

where $x = (1 + \Delta)/2$ and $y = (1 - \Delta)/2$, and the corresponding ground state energy is

$$
E_0 = -\frac{z}{2}NS^2 + \frac{zS}{2}\sum_{\mathbf{k}} \left( 1 + y\gamma_k \right) \times \left( \sqrt{1 - x^2\gamma_k^2}/(1 + y\gamma_k^2) - 1 \right).
$$

(20)

Within the spin-wave theory framework, we calculate the spin correlation function $C_{ij}^{SW}$ and hence the concurrence $C_{ij}$ of the model in two and three dimensions. Our results are shown in Figs. 1 and 2 respectively. We also
show results obtained from the exact diagonalization of the $XXZ$ model on finite square lattices. The trend as function of lattice size is clear. It is interesting to see that, in both cases, the concurrences $C_{ij}$ of the $XXZ$ model not only have their maximal value at the critical point $\Delta = 1$, but also show discontinuities in their first derivative with respect to $\Delta$ at the transition point. This behavior is quite different from the one-dimensional case (Eq. 10), as we expected. We attribute this difference to the existence of the magnetic long-range orders in the system with $d \geq 2$.

As we have seen, the concurrence $C_{ij}$ is closely related to the ground state energy of the model. As a result, any singularity in the ground state energy may be inherited by the concurrence $C_{ij}$. On the other hand, on a finite $d$-dimensional simple cubic lattice, the ground state of the antiferromagnetic $XXZ$ model is non-degenerate for $\Delta \in (-\infty, \infty)$ [10]. Therefore, the ground state energy $E_0(\Lambda, \Delta)$ as well as the concurrence $C_{ij}$ are analytical functions of $\Delta$, regardless of the dimensionality of the lattice. However, it is no longer true in the thermodynamic limit. For the one-dimensional $XXZ$ model, it is well known that its ground state in both $\Delta < 1$ and $\Delta > 1$ regions does not have magnetic long-range order. Therefore, we do not expect a dramatic change in the ground state energy $E_0$ taking place at $\Delta = 1$. Consequently, the concurrence will behave more or less like itself on a finite lattice. However, in two and three dimensions, the ground state energy of the system develops a cusp at the transition point in the thermodynamic limit [21]. This phenomenon can be understood by the picture of the first excited-energy levels crossing at $\Delta = 1$, required by the existence of magnetic long-range order [22]. Therefore, a singularity inherited by the concurrence at the transition point, is expected to appear, as shown by our calculations.

In summary, we have studied the ground state two-spin entanglement, as measured by the concurrence, in the $d$-dimensional $XXZ$ model. We gave a rigorous proof that the ground state concurrence in the $XXZ$ model reaches maximum at the isotropic point. We extended our previous studies in one dimension [7] to two and three dimensions by using the spin-wave theory and exact diagonalization technique. The use of the spin-wave theory is justified by the existence of magnetic long-range order in the $XXZ$ model for dimensionality $d \geq 2$. We found that the concurrence in two- and three-dimensional $XXZ$ models also reaches maximum at the isotropic point $\Delta = 1$. Unlike the one dimension case, the concurrence shows cusp-like behavior around the critical point, and its first derivative is not continuous in the vicinity of the critical point.

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[1] A. Einstein, B. Podolsky, and N. Rosen, Phys. Rev. 47, 777 (1935).
[2] M. A. Nielsen and I. L. Chuang, Quantum Computation and Quantum Information (Cambridge University Press, Cambridge, 2000).
[3] A. Osterloh, Luigi Amico, G. Falci and Rosario Fazio, Nature 416, 608 (2002).
[4] T. J. Osborne and M.A. Nielsen, Phys. Rev. A 66, 032110 (2002).
[5] I. Bose and E. Chattopadhyay, Phys. Rev. A 66, 062320 (2002).
[6] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. 90, 227902 (2003); J. I. Latorre, E. Rico, and G. Vidal, quant-ph/0304098 (2003).
[7] S. J. Gu, H. Q. Lin, and Y. Q. Li, Phys. Rev. A 68, 042330 (2003).
[8] J. Vidal, G. Palacios, and R. Mosseri, Phys. Rev. A 69, 022107 (2004); J. Vidal, R. Mosseri, J. Dukelsky, Phys. Rev. A 69, 054101 (2004).
[9] L. A. Wu, M. S. Sarandy, and D. A. Lidar, arXiv: quant-ph/0407056.
[10] M. F. Yang, arXiv: quant-ph/0407226.
[11] Y. Chen, P. Zanardi, Z. D. Wang, and F. C. Zhang, arXiv: quant-ph/0407228.
[12] S. Sachdev, Quantum Phase Transitions, (Cambridge University Press, Cambridge, UK, 2000).
[13] S. Hill and W. K. Wootters, Phys. Rev. Lett. 78, 5022 (1997); W. K. Wootters, Phys. Rev. Lett. 80, 2245 (1998).
[14] Olav F. Syljuasen, arXiv:quant-ph/0312101.
[15] E. Lieb and D. Mattis, J. Math. Phys. 3, 749 (1962).
[16] I. Affleck and E. Lieb, Lett. Math. Phys. 12, 57 (1986).
[17] K. M. O’Connor and W. K. Wootters, Phys. Rev. A 63, 052302 (2001).
[18] X. Wang, and P. Zanardi, Phys. Lett. A 301, 1(2002).
[19] J. Franklin, Matrix Theory (Prentice Hall, New Jersey, 1968).
[20] A. W. Sandvik, Phys. Rev. B 56, 11678 (1997).
[21] H. Q. Lin, J. S. Flynn, and D. D. Betts, Phys. Rev. B 64, 214411 (2001).
[22] J. E. Hirsch, and S. Tang, Phys. Rev. B 40, 4769 (1989).
[23] Zheng Weihong, J. Oittmaa, and C. J. Hamer, Phys. Rev. B 43, 8321 (1991).
[24] F. J. Dyson, E. H. Lieb, and B. Simon, J. Stat. Phys. 18, 335 (1978); E. J. Neves and J. F. Perez, Phys. Lett. A114, 331 (1986); T. Kennedy, E. Lieb, and B. S. Shastry, J. Stat. Phys. 53, 1019 (1988).
[25] G. S. Tian and H. Q. Lin, Phys. Rev. B 67, 245105 (2003).