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 $d \geqslant 2$, 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 nonlocal connotations [1]. Recently, many physicists have made great efforts to understand the quantum entanglement in the ground states of some many-body spin models [2–10]. One expects that a thorough investigation on the entanglement in these systems will provide additional insight into the quantum phase transition in these systems [11]. For example, Osterloh *et al.* [2] studied the concurrence, a measure of entanglement of two qubits [12], between two spins located on a pair of nearest-neighbor sites in the transverse-field Ising model [3]. They found that this quantity shows singularity and obeys the scaling law in the vicinity of the quantum phase transition point of the system. On the other hand, for other models, such as the antiferromagnetic *XXZ* chain, the concurrence behaves in a completely different way [6]. As shown by Ref. [6], the concurrence is a continuous function of the anisotropic parameter and reaches its maximum at the transition point. Therefore, in both cases, one observes that the concurrence itself manifests interesting behaviors at the quantum phase transition points. However, we should emphasize that, such behaviors alone may not always signal a quantum phase transition, as pointed out by the authors of Refs. [8,9].

In Ref. [6], we studied extensively nearest-neighbor spin entanglement in the antiferromagnetic *XXZ* chain. By applying results derived from the Bethe ansatz solution of the model, we showed clearly that the concurrence between two spins located on a pair of nearest-neighbor sites in the system is a continuous function of the anisotropic coupling parameter and becomes maximal at the isotropic Heisenberg point. In this paper, we continue our discussions on this issue. Our main purpose is to show that some fundamental properties of the *XXZ* model, such as nondegeneracy and concavity of the ground-state energy of the system at the phase transition point, have strong effects on the behavior of the concurrence. Therefore, we expect that the same scenario will appear in a wide class of localized spin models, such as the spin ladder model and, in particular, the *XXZ* model in higher dimensions [13]. 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, we study the concurrence as a function of the anisotropic parameter on a finite lattice by the exact diagonalization technique. For the infinite system, we use the spin-wave theory, which is justified by the existence of magnetic long-range order (LRO) in the *XXZ* model, to show that a cusplike behavior of the concurrence develops in the thermodynamic limit when the dimensionality of the lattice $d \geqslant 2$.

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

$$\hat{H}_{XXZ} = \sum_{\langle \mathbf{ij} \rangle} (\hat{S}_\mathbf{i}^x \hat{S}_\mathbf{j}^x + \hat{S}_\mathbf{i}^y S_\mathbf{j}^y + \Delta \hat{S}_\mathbf{i}^z \hat{S}_\mathbf{j}^z), \qquad (1)$$

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

The conservation of $\hat{S}_{\text{total}}^z$ implies also that, with respect to the standard basis vectors $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, and $|\downarrow\downarrow\rangle$, the reduced density matrix of two spins on a pair of nearest-neighbor lattice sites **i** and **j** can be put into the following block-diagonal form:

$$\hat{\rho}_{\mathbf{ij}} = \begin{pmatrix} u^+ & 0 & 0 & 0 \\ 0 & w_1 & z & 0 \\ 0 & z^* & w_2 & 0 \\ 0 & 0 & 0 & u^- \end{pmatrix}. \tag{2}$$

Following Ref. [12], the concurrence of this two-qubit system is defined by

$$C_{\mathbf{ij}} = \max(0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}), \tag{3}$$

where $\lambda_1 \geqslant \lambda_2 \geqslant \lambda_3 \geqslant \lambda_4 \geqslant 0$ are the eigenvalues of the semi-positive definite matrix

$$\rho_{\mathbf{ij}}\tilde{\rho}_{\mathbf{ij}} \equiv \rho_{\mathbf{ij}}(\sigma_{\mathbf{i}}^y \otimes \sigma_{\mathbf{j}}^y \rho_{\mathbf{ij}}^* \sigma_{\mathbf{i}}^y \otimes \sigma_{\mathbf{j}}^y). \tag{4}$$

An important observation is that there exists a one-to-one correspondence between $C_{\mathbf{ij}}$ and the entanglement formation of these spins. Consequently, $C_{\mathbf{ij}}$ can be used as a measurement of their entanglement [12]. Furthermore, in terms of the correlation functions $G_{\mathbf{ij}}^{\alpha\alpha} = \langle \hat{S}_{\mathbf{i}}^\alpha \hat{S}_{\mathbf{j}}^\alpha \rangle$, $\alpha = x, y, z$, $C_{\mathbf{ij}}$ can be explicitly written as [16,17]

$$C_{\mathbf{ij}} = 2\max\left(|G_{\mathbf{ij}}^{xx} + G_{\mathbf{ij}}^{yy}| - G_{\mathbf{ij}}^{zz} - \frac{1}{4}, 0\right). \tag{5}$$

We notice that the functions $G_{\mathbf{ij}}^{\alpha\alpha}$ in Eq. (5) represent actually the total correlation between the spins at sites **i** and **j**. On the other hand, the constant 1/4 is the maximal absolute value of their longitudinal (or classical) correlation. Therefore, being the difference of these quantities, $C_{\mathbf{ij}}$ can be thought of as the remaining "quantum correlation" between them. Naturally, one would like to study the behavior of $C_{\mathbf{ij}}$ near the quantum phase transition point $\Delta = 1$. It deepens our understanding on such transitions.

First, we show that, on any finite d-dimensional bipartite lattice, $C_{\mathbf{ij}}$ takes on its maximum at point $\Delta = 1$. By the variational principle, it is easy to see that all the spin correlations functions $G_{\mathbf{ij}}^{\alpha\alpha}$ in Eq. (5) are negative. Thus, we have

$$\begin{aligned} C_{\mathbf{ij}} &= \left(-G_{\mathbf{ij}}^{xx} - G_{\mathbf{ij}}^{yy} - \frac{1}{4} - G_{\mathbf{ij}}^{zz}\right) \\ &= \left(-\epsilon_{\mathbf{ij}}^0(\Lambda, \Delta) - \frac{1}{4} + (\Delta - 1)G_{\mathbf{ij}}^{zz}\right), \end{aligned} \tag{6}$$

where $\epsilon_{\mathbf{ij}}^0(\Lambda, \Delta) = E_0(\Lambda, \Delta)/N_B$ (N_B is the number of bonds in the lattice) is the ground-state energy density per bond. Furthermore, since all quantities in $C_{\mathbf{ij}}$ are analytical functions of the parameter Δ, we are allowed to take derivatives of it with respect to Δ. In particular, after taking the first-order derivative of $C_{\mathbf{ij}}$, we obtain

$$\frac{\partial C_{\mathbf{ij}}}{\partial \Delta} = 2\left(-\frac{\partial \epsilon_{\mathbf{ij}}^0(\Lambda, \Delta)}{\partial \Delta} + G_{\mathbf{ij}}^{zz} + (\Delta - 1)\frac{\partial G_{\mathbf{ij}}^{zz}}{\partial \Delta}\right). \tag{7}$$

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 $\partial \epsilon_{\mathbf{ij}}^0(\Lambda, \Delta)/\partial \Delta$, which equals $G_{\mathbf{ij}}^{zz}$. Therefore, we finally obtain

$$\frac{\partial C_{\mathbf{ij}}}{\partial \Delta} = 2(\Delta - 1)\frac{\partial G_{\mathbf{ij}}^{zz}}{\partial \Delta} = 2(\Delta - 1)\frac{\partial^2 \epsilon_{\mathbf{ij}}^0(\Lambda, \Delta)}{\partial \Delta^2}. \tag{8}$$

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 $C_{\mathbf{ij}}$ and the concurrence does not have another 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 Δ. By the variational principle [18], we know that, for any two parameters Δ_1 and Δ_2, the inequality

$$E_0[\Lambda, \lambda\Delta_1 + (1-\lambda)\Delta_2] \geqslant \lambda E_0(\Lambda, \Delta_1) + (1-\lambda)E_0(\Lambda, \Delta_2), \tag{9}$$

where $0 \leqslant \lambda \leqslant 1$, holds true for the ground-state energy $E_0(\Lambda, \Delta)$. In particular, when $E_0(\Lambda, \Delta)$ is differentiable with respect to Δ, the inequality (9) is equivalent to

$$\frac{\partial^2 E_0(\Lambda, \Delta)}{\partial \Delta^2} \leqslant 0. \tag{10}$$

Consequently, we have also $\partial^2 \epsilon_{\mathbf{ij}}^0(\Lambda, \Delta)/\partial \Delta^2 \leqslant 0$. Now, let us take the derivative of Eq. (8) again with respect to Δ. It yields

$$\left.\frac{\partial^2 C_{\mathbf{ij}}}{\partial \Delta^2}\right|_{\Delta=1} = 2\left.\frac{\partial^2 \epsilon_{\mathbf{ij}}^0(\Lambda, \Delta)}{\partial \Delta^2}\right|_{\Delta=1} \leqslant 0. \tag{11}$$

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 $C_{\mathbf{ij}}$. For that purpose, we notice that the inequality (10) 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 Δ increases from $-\infty$ to ∞, quantity $\langle \hat{S}_{\mathbf{i}}^z \hat{S}_{\mathbf{i}}^z \rangle = \partial \epsilon_{\mathbf{ij}}^0(\Lambda, \Delta)/\partial \Delta$ becomes more and more negative. Consequently, the product on the right-hand side of Eq. (8) cannot be zero at any point except $\Delta = 1$. That completes our discussion on the general behavior of the concurrence $C_{\mathbf{ij}}$ 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 $J_\perp = 0$.

In the following, we shall discuss the analyticity of the concurrence in the vicinity of phase transition. In Ref. [6], by using the Bethe ansatz solution of the one-dimensional XXZ chain, we obtained the explicit expression of the concurrence near the isotropic point

$$C_{i,i+1} = C_0 - C_1(\Delta - 1)^2, \tag{12}$$

where C_0 and C_1 are two real constants. Therefore, the concurrence of the one-dimensional XXZ chain is a differentiable function of Δ 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 [19]. 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 16×16, Sandvik [20] 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 σ 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 [21] studied the *XXZ* model on square lattices and obtained various quantities as functions of the anisotropic parameter Δ for the infinite system. Two conclusions from previous work [20–23] are relevant to the present study: (i) results obtained from the spin-wave theory are qualitatively correct and quite accurate, usually within 3% as compared with exact solution on finite lattices; (ii) derivatives of the ground-state energy with respect to the anisotropic parameter Δ are not continuous at the Heisenberg point $\Delta=1$; for example, see Fig. 3 in Ref. [21]. This conclusion is consistent with the belief that there exists antiferromagnetic long-range order in the d-dimensional *XXZ* model for $d\geqslant 2$. In other words, the correlation function $\langle \hat{S}_{\mathbf{i}}^{\alpha}\hat{S}_{\mathbf{i+r}}^{\alpha}\rangle$ does not vanish as $\mathbf{r}\to\infty$. Theoretically, the existence of the LRO in $d\geqslant 3$ dimensions has been rigorously proven [24], while for $d=2$ most numerical studies support it. Based on these conclusions, we apply the spin-wave theory to calculate the concurrence $C_{\mathbf{ij}}$ 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-Primarkoff transformation

$$\hat{S}_{\mathbf{i}}^{+}=\sqrt{2S}(1-\hat{n}_{\mathbf{i}}/2S)^{1/2}\hat{a}_{\mathbf{i}}\simeq\sqrt{2S}(1-\hat{n}_{\mathbf{i}}/4S)\hat{a}_{\mathbf{i}},$$

$$\hat{S}_{\mathbf{i}}^{-}=\sqrt{2S}\hat{a}_{\mathbf{i}}^{\dagger}(1-\hat{n}_{\mathbf{i}}/2S)^{1/2}\simeq\sqrt{2S}\hat{a}_{\mathbf{i}}^{\dagger}(1-\hat{n}_{\mathbf{i}}/4S),$$

$$\hat{S}_{\mathbf{i}}^{z}=S-\hat{a}_{\mathbf{i}}^{\dagger}\hat{a}_{\mathbf{i}}, \tag{13}$$

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

$$\hat{H}_{XXZ}/\Delta\simeq\sum_{\langle\mathbf{ij}\rangle}[-S^2+S(\hat{a}_{\mathbf{i}}^{\dagger}\hat{a}_{\mathbf{i}}+\hat{a}_{\mathbf{j}}^{\dagger}\hat{a}_{\mathbf{j}})+xS(\hat{a}_{\mathbf{i}}\hat{a}_{\mathbf{j}}+\hat{a}_{\mathbf{i}}^{\dagger}\hat{a}_{\mathbf{j}}^{\dagger})], \tag{14}$$

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

$$\hat{H}_{XXZ}/\Delta=-\frac{z}{2}NS^2+zS\sum_{\mathbf{k}}\hat{H}(\mathbf{k}), \tag{15}$$

where z is the coordination number of the lattice and

$$\hat{H}(\mathbf{k})=\hat{a}_{\mathbf{k}}^{\dagger}\hat{a}_{\mathbf{k}}+\frac{x\gamma_{\mathbf{k}}}{2}(\hat{a}_{\mathbf{k}}\hat{a}_{-\mathbf{k}}+\hat{a}_{-\mathbf{k}}^{\dagger}\hat{a}_{\mathbf{k}}^{\dagger}) \tag{16}$$

with $\gamma_{\mathbf{k}}=(2/z)\Sigma_{m=1}^{d}\cos k_m$. By applying the Bogoliubov transformation

$$\hat{a}_{\mathbf{k}}=u_{\mathbf{k}}\hat{c}_{\mathbf{k}}-v_{\mathbf{k}}\hat{c}_{-\mathbf{k}}^{\dagger},$$

$$\hat{a}_{\mathbf{k}}^{\dagger}=-v_{\mathbf{k}}\hat{c}_{-\mathbf{k}}+u_{\mathbf{k}}\hat{c}_{\mathbf{k}}^{\dagger}, \tag{17}$$

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

$$\hat{H}(\mathbf{k})=v_{\mathbf{k}}^2-x\gamma_{\mathbf{k}}u_{\mathbf{k}}v_{\mathbf{k}}+(u_{\mathbf{k}}^2+v_{\mathbf{k}}^2-2xu_{\mathbf{k}}v_{\mathbf{k}}\gamma_{\mathbf{k}})\hat{c}_{\mathbf{k}}^{\dagger}\hat{c}_{\mathbf{k}}, \tag{18}$$

where the $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ satisfy the following constraint conditions:

$$u_{\mathbf{k}}^2-v_{\mathbf{k}}^2=1,$$

$$\frac{x\gamma_{\mathbf{k}}}{2}(u_{\mathbf{k}}^2+v_{\mathbf{k}}^2)-u_{\mathbf{k}}v_{\mathbf{k}}=0. \tag{19}$$

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

$$E_0(\Delta>1)=-\frac{z}{2}NS^2+\frac{zS}{2}\sum_{\mathbf{k}}(\sqrt{1-x^2\gamma_{\mathbf{k}}^2}-1). \tag{20}$$

By a 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 form

$$\hat{H}(\mathbf{k})=(1+y\gamma_{\mathbf{k}})v_{\mathbf{k}}^2-x\gamma_{\mathbf{k}}u_{\mathbf{k}}v_{\mathbf{k}}+[(1+y\gamma_{\mathbf{k}})(u_{\mathbf{k}}^2+v_{\mathbf{k}}^2)-2xu_{\mathbf{k}}v_{\mathbf{k}}\gamma_{\mathbf{k}}]\hat{c}_{\mathbf{k}}^{\dagger}\hat{c}_{\mathbf{k}}, \tag{21}$$

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

$$E_0=-\frac{z}{2}NS^2+\frac{zS}{2}\sum_{\mathbf{k}}(1+y\gamma_{\mathbf{k}})\times(\sqrt{1-x^2\gamma_{\mathbf{k}}^2/(1+y\gamma_{\mathbf{k}})^2}-1). \tag{22}$$

Within the spin-wave theory framework, we calculate the spin correlation function $G_{\mathbf{ij}}^{zz}$ and hence the concurrence $C_{\mathbf{ij}}$ 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 a function of lattice size is clear. It is interesting to see that, in both cases, the concurrences $C_{\mathbf{ij}}$ 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 Δ at the transition point. This behavior is quite different from the one-dimensional case [Eq. (12)], as we expected. We attribute

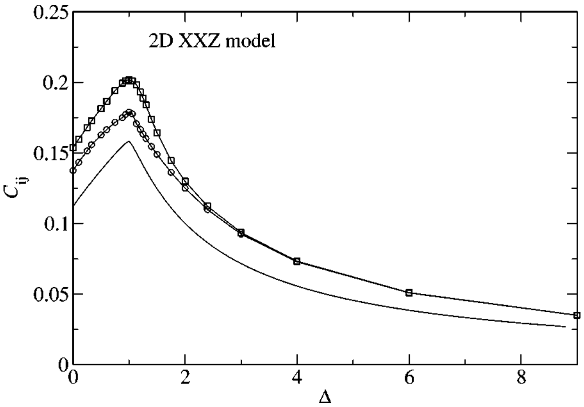

FIG. 1. The concurrence $C_{\mathbf{ij}}$ of the two-dimensional *XXZ* model as a function of Δ ($=J_z/J_x$). In the figure, the dotted lines are obtained from the exact diagonalization for 4×4 (square) and 6×6 (circle) square lattices respectively; the solid line is from spin-wave theory.

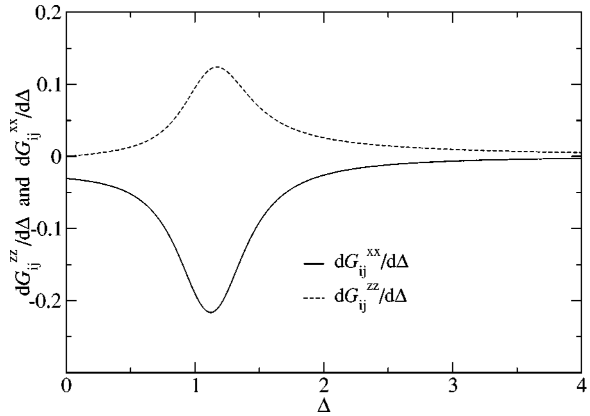

FIG. 3. The first derivative of the correlation function of the two-dimensional *XXZ* model as a function of Δ ($=J_z/J_x$) for a 4×4 square lattice.

this difference to the existence of the magnetic long-range order in the system with $d\geqslant2$.

As we have seen, the concurrence $C_{\mathbf{ij}}$ 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 [8]. On the other hand, on a finite d-dimensional simple cubic lattice, the ground state of the antiferromagnetic *XXZ* model is nondegenerate for $\Delta\in(-1,\infty)$ [15]. Therefore, the ground-state energy $E_0(\Lambda,\Delta)$ as well as the concurrence $C_{\mathbf{ij}}$ are analytical functions of Δ, 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 the $\Delta<1$ and $\Delta>1$ regions does not have magnetic long-range order. Therefore, the local properties of the system, such as energy, spin-spin correlations of the nearest neighbors, etc., are not affected by those spins far away. So 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].

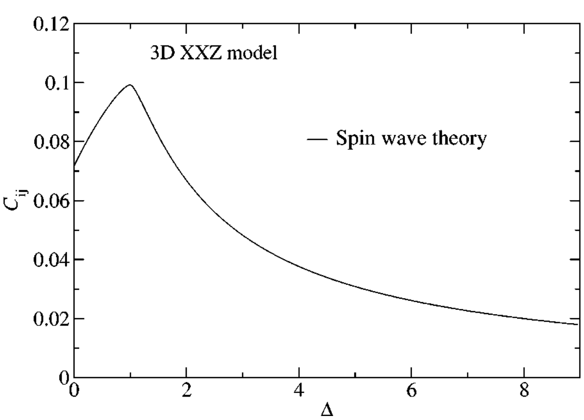

FIG. 2. The concurrence $C_{\mathbf{ij}}$ of the three-dimensional *XXZ* model as a function of Δ ($=J_z/J_x$).

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 [25]. Furthermore, due to the existence of long-range correlations, one expects that the properties, such as entanglement, of the localized spin pairs are greatly affected by the collective modes of the whole system. In particular, it is well known that, in general, the long-range order makes the change of these quantities at the transition point more abrupt [11]. Therefore, the singular behavior of the concurrence at the transition point should be expected. Our calculation confirms this speculation.

A further remark is in order. Conventionally, one identifies the phase boundary of a many-body system by studying divergence of the corresponding correlation functions in the thermodynamic limit. On the other hand, as far as numerical calculations are concerned, investigations on large-size samples are limited by the current computation facilities. As a result, one needs to do rather sophisticated calculations to determine the exact transition point by numerics. For instance, in Fig. 3, we draw the calculated curves of the first derivative of correlation functions $G_{\mathbf{ij}}^{xx}(\Delta)$ and $G_{\mathbf{ij}}^{zz}(\Delta)$ with respect to Δ for the *XXZ* model on a 4×4 lattice. It is clear that both the extreme points do not coincide with $\Delta=1$, although they do approach to it as the size of sample increases.

On the other hand, as expressed in Eq. (6), the concurrence $C_{\mathbf{ij}}$ is a function of these correlation functions. As proven above, on any finite bipartite lattice, this quantity reaches its maximum at point $\Delta=1$. That makes identification of the phase transition point much easier. By studying several concrete examples, we found that this observation holds true for other interesting systems, such as the spin ladder model, too. That strongly suggests that one can determine the quantum phase transition points of a specific many-body system by finding out the singular points of particle entanglement in its ground state. Moreover, it also provides us with further information on the quantum correlations among particles in the system.

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 a maximum at the isotropic point. We extended our previous studies in one dimension [6] 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 $d \geqslant 2$. We found that the concurrence in two- and three-dimensional *XXZ* models also reaches a maximum at the isotropic point $\Delta = 1$. Unlike the one-dimensional case, the concurrence shows cusplike behavior around the critical point, and its first derivative is not continuous in the vicinity of the critical point.

Note added: Recently, we received work from Dr. M. F. Yang prior to publication [9]. Some of our results were also obtained by him.

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