Thermal and ground-state entanglement in Heisenberg *XX* qubit rings

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We study the entanglement of thermal and ground states in the Heisenberg *XX* qubit rings with a magnetic field. A general result is found that for even-number rings, pairwise entanglement between nearest-neighbor qubits is independent of both the sign of exchange interaction constants and the sign of magnetic fields. As an example we study the entanglement in the four-qubit model and find that the ground state of this model without magnetic fields is shown to be a four-body maximally entangled state measured by the square N-bit concurrence.

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Quantum entanglement is an important prediction of quantum mechanics and constitutes indeed a valuable resource in quantum information processing [1]. Much efforts have been devoted to the study and characterization of it. Very recently one kind of natural entanglement, the thermal entanglement [2–7], has been proposed and investigated. The investigations of this type of entanglement, ground-state entanglement [8,9] in quantum spin models, and relations [10,11] between quantum phase transition [12] and entanglement provide a bridge between the quantum information theory and condensed-matter physics.

Consider a thermal equilibrium state in a canonical ensemble. In this situation the system state is described by the Gibb's density operator $\rho_T = \exp(-H/kT)/Z$, where $Z = \mathrm{tr}[\exp(-H/kT)]$ is the partition function, H is the system Hamiltonian, k is Boltzmann's constant that we henceforth will take equal to 1, and T is the temperature. As ρ_T represents a thermal state, the entanglement in the state is called *thermal entanglement* [2]. In a recent paper [6] we showed that in the isotropic Heisenberg XXX model the thermal entanglement is completely determined by the partition function and is directly related to the internal energy. In general, the entanglement cannot be determined only by the partition function.

In this Brief Report, we consider a physical Heisenberg XX N-qubit ring with a magnetic field and aim to obtain some general results about the thermal and ground-state entanglement. We consider a four-qubit model as an example and examine in detail the properties of entanglement. Both the pairwise and many-body entanglements are considered.

In our model the qubits interact via the following Hamiltonian [13]:

$$H(J,B) = J\sum_{i=1}^{N} (\sigma_{ix}\sigma_{i+1x} + \sigma_{iy}\sigma_{i+1y}) + B\sum_{i=1}^{N} \sigma_{iz}, \tag{1}$$

where $\vec{\sigma}_i = (\sigma_{ix}, \sigma_{iy}, \sigma_{iz})$ is the vector of Pauli matrices, J is the exchange constant, and B is the magnetic field. The positive and negative J correspond to the antiferromagnetic (AFM) and ferromagnetic (FM) cases, respectively. We assume periodic boundary conditions, i.e., $N+1 \equiv 1$. Therefore the model has the symmetry of translational invariance.

It is easy to check that the commutator $[H,S_z]=0$, (rotation symmetry about the z axis) which guarantees that reduced density matrix $\rho_{12} = \mathrm{tr}_{3,4,\ldots,N}(\rho_T)$ of two nearest-neighbor qubits, say qubit 1 and 2, for the thermal state ρ_T has the form [8]

$$\rho_{12} = \begin{pmatrix} u_+ & 0 & 0 & 0 \\ 0 & w & z & 0 \\ 0 & z & w & 0 \\ 0 & 0 & 0 & u_- \end{pmatrix} \tag{2}$$

in the standard basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$. Here $|ij\rangle \equiv |i\rangle \otimes |j\rangle (i,j=0,1)$, $|0\rangle$ ($|1\rangle$) denotes the state of spin-up (-down), and $S_z = \sum_{i=1}^{N} \sigma_{iz}/2$ are the collective spin operators. The Hamiltonian is invariant under the transformation $\Pi_{n=1}^{N/2} S_{n,N-n+1}$, where S_{ij} is the swap operator for qubits i and j. This is reflection symmetry which implies that the matrix element z is a real number. For any operator A_{12} acting on qubits 1 and 2, we have the relation

$$\mathrm{tr}_{12}(A_{12}\rho_{12}) = \mathrm{tr}_{1,2,\ldots,N}(A_{12}\rho_T). \tag{3}$$

Then the reduced density matrix ρ_{12} is directly related to various correlation functions $G_{\alpha\beta} = \langle \sigma_{1\alpha}\sigma_{2\beta} \rangle = \mathrm{tr}_{1,\ldots,N}(\sigma_{1\alpha}\sigma_{2\beta}\rho_T)$ $(\alpha = x,y,z)$. Precisely the matrix elements can be written in terms of the correlation functions and the magnetization $M = \mathrm{tr}(\sum_{i=1}^{N} \sigma_{iz}\rho_T)$ as

$$\begin{aligned} u_+ &= \mathrm{tr}_{1,\ldots,N}(|00\rangle\langle 00|) = \tfrac{1}{4}(1 + 2\bar{M} + G_{zz}), \\ u_- &= \mathrm{tr}_{1,\ldots,N}(|11\rangle\langle 11|) = \tfrac{1}{4}(1 - 2\bar{M} + G_{zz}), \\ z &= \mathrm{tr}_{1,\ldots,N}(|01\rangle\langle 10|) = \tfrac{1}{4}(G_{xx} + G_{yy}), \end{aligned} \tag{4}$$

where $\bar{M} = M/N$ is the magnetization per site. In deriving the above equation, we have used the translational invariance of the Hamiltonian.

Due to the fact $[H,S_z]=0$ one has $G_{xx} = G_{yy}$. Then, the concurrence [14] quantifying the entanglement of two qubits is readily obtained as [8]

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$$C=\max\left[0,\left|G_{xx}\right|-\frac{1}{2}\sqrt{(1+G_{zz})^2-4\bar{M}^2}\right], \tag{5}$$

which is determined by the correlation function G_{xx},G_{zz}, and the magnetization. In the literature there are a lot of results on correlation functions [15] in various quantum spin models, and they may be used for the calculations of entanglement.

By using the translational invariance of the Hamiltonian and the rotational symmetry about the z axis, we find a useful relation

$$G_{xx}=(\bar{U}-B\bar{M})/(2J), \tag{6}$$

where $\bar{U}=U/N$ is the internal energy per site and U is the internal energy. From the partition function we can obtain the internal energy and the magnetization through the well-known relations

$$U=-\frac{1}{Z}\frac{\partial Z}{\partial \beta},M=-\frac{1}{Z\beta}\frac{\partial Z}{\partial B}, \tag{7}$$

where $\beta=1/T$. As a combination of Eqs. (6) and (7) the correlation function G_{xx} is solely determined by the partition function. Therefore the concurrence can be obtained from the partition function and the correlation function G_{zz}. We see that the partition function itself is not sufficient for determining the entanglement.

Except for the symmetries used in the above discussions there are also other symmetries in our model. Consider the operator $\Lambda_x\equiv\sigma_{1x}\otimes\sigma_{2x}\otimes\cdots\otimes\sigma_{Nx}$ satisfing $\Lambda_x^2=1$. We have the commutator $[\sigma_{i\alpha}\sigma_{i+1\alpha},\Lambda_x]=0$ and anticommutator $[\sigma_{iz},\Lambda_x]_+=0$. Then we immediately obtain

$$\begin{aligned}G_{\alpha\alpha}&=\mathrm{tr}\{\Lambda_x\sigma_{1\alpha}\sigma_{2\alpha}\exp[-\beta H(J,B)]\Lambda_x\}/Z\\&=\mathrm{tr}\{\sigma_{1\alpha}\sigma_{2\alpha}\exp[-\beta H(J,-B)]\}/Z,\end{aligned}$$

$$\begin{aligned}\bar{M}&=\mathrm{tr}\{\Lambda_x\sigma_{1z}\exp[-\beta H(J,B)]\Lambda_x\}/Z\\&=-\mathrm{tr}\{\sigma_{1z}\exp[-\beta H(J,-B)]\}/Z.\end{aligned}$$

These equations tell us that the correlation function $G_{\alpha\alpha}$ and the square of the magnetization is invariant under the transformation $B\rightarrow -B$. From Eq. (5) and the invariance of $G_{\alpha\alpha}$ and $\bar{M}^2$ we find the following Proposition.

Proposition 1. The concurrence is invariant under the transformation $B\rightarrow -B$.

The proposition shows that the pairwise thermal entanglement of the nearest-neighbor qubits is independent of the sign of the magnetic field. And it is valid for both the even and the odd number of qubits.

In Ref. [3], we observe an interesting result that the pairwise thermal entanglement for two-qubit XX model with a magnetic field is independent of the sign of the exchange constant J. Now we generalize this result to the case of arbitrary even-number qubits.

For the case of even-number qubits we have

$$H(-J,B)=\Lambda_z H(J,B)\Lambda_z,$$

$$\Lambda_z=\sigma_{1z}\otimes\sigma_{3z}\otimes\cdots\otimes\sigma_{N-1z}.$$

The transformation Λ_z changes the sign of the exchange constant J. Note that the definition of Λ_z is different from that of Λ_x. It is straightforward to prove

$$G_{xx}=\mathrm{tr}(\Lambda_z\sigma_{1x}\sigma_{2x}e^{-\beta H(J,B)}\Lambda_z)=-\mathrm{tr}(\sigma_{1x}\sigma_{2x}e^{-\beta H(-J,B)}),$$

$$G_{zz}=\mathrm{tr}(\Lambda_z\sigma_{1z}\sigma_{2z}e^{-\beta H(J,B)}\Lambda_z)=\mathrm{tr}(\sigma_{1z}\sigma_{2z}e^{-\beta H(-J,B)}),$$

$$\bar{M}=\mathrm{tr}(\sigma_{1z}e^{-\beta H(-J,B)}).$$

From these equations we see that the absolute value $|G_{xx}|$, the correlation function G_{zz}, and the magnetization are invariant under the transformation $J\rightarrow -J$. Hence from Eq. (5) and Proposition 1 we arrive at the following Proposition.

Proposition 2. For the even-number XX model with a magnetic field the pairwise thermal entanglement of nearest-neighbor qubits is independent of the sign of exchange constant J and the sign of magnetic field B.

The proposition shows that the entanglement of AFM qubit rings is the same as that of FM rings.

Now we consider the case of no magnetic fields. Then the magnetization will be zero and Eq. (5) reduces to $C=\frac{1}{2}\max(0,|\bar{U}/J|-G_{zz}-1)$. We can prove that the internal energy is always negative. First, from the traceless property of the Hamiltonian, it is immediate to check that

$$\lim_{T\rightarrow\infty}U=\lim_{T\rightarrow\infty}\frac{\sum_n E_n e^{-E_n/T}}{\sum_n e^{-E_n/T}}=0, \tag{8}$$

where E_n is the eigenvalue of the Hamiltonian H. In this limit the correlation function G_{xx} and the magnetization M are also zero. Further from the fact that

$$\partial U/\partial T=(\langle H^2\rangle-\langle H\rangle^2)/T^2=(\Delta H)^2/T^2>0 \tag{9}$$

we conclude that U is always negative. Then we arrive at the following Proposition.

Proposition 3. The concurrence of the nearest-neighbor qubits in the Heisenberg XX model without a magnetic field is given by

$$C=\begin{cases}\frac{1}{2}\max[0,-\bar{U}/J-G_{zz}-1] & \text{for AFM,}\\ \frac{1}{2}\max[0,\bar{U}/J-G_{zz}-1] & \text{for FM.}\end{cases} \tag{10}$$

From the proposition we know that even for the case of no magnetic fields the partition function itself cannot determine the entanglement. In the limit of $T\rightarrow 0$, the above equation reduces to

$$C=\begin{cases}\frac{1}{2}\max\left[0,-\frac{E^{(0)}}{NJ}-G_{zz}^{(0)}-1\right] & \text{for AFM},\\ \frac{1}{2}\max\left[0,\frac{E^{(0)}}{NJ}-G_{zz}^{(0)}-1\right] & \text{for FM},\end{cases} \tag{11}$$

where $E^{(0)}$ is the ground-state energy and $G_{zz}^{(0)}$ is the correlation function on the ground state. Therefore the ground-state pairwise entanglement of the system is determined by both the ground-state energy and the correlation function $G_{zz}^{(0)}$. Next we consider a four-qubit XX model as an example.

To study the pairwise entanglement we need to solve the eigenvalue problems of the four-qubit Hamiltonian. We work in the invariant subspace spanned by vectors of fixed number r of reversed spins. The subspace $r=0$ $(r=4)$ is trivially containing only one eigenstate $|0000\rangle$ $(|1111\rangle)$ with eigenvalue $4B$ $(-4B)$. The subspace $r=1$ is four dimensional. The corresponding eigenvectors and eigenvalues are given by

$$|k\rangle=\frac{1}{2}\sum_{n=1}^{4}\exp(-ink\pi/2)|n\rangle_0(k=0,\ldots,3), \tag{12}$$

and $4J\cos(k\pi/2)+2B$, respectively. Here the "number state" $|n\rangle_0=\mathcal{T}^{n-1}|1\rangle_0$, $|1\rangle_0=|1000\rangle$, and $\mathcal{T}$ is the cyclic right shift operator that commutes with the Hamiltonian H [16]. Due to the fact that H commutes Λ_x, $|k\rangle'=\Lambda_x|k\rangle$ is also a eigenstate with eigenvalue $4J\cos(k\pi/2)-2B$. The states $|k\rangle$ and $|k\rangle'$ are the so-called W states [17] whose corresponding concurrence is 1/2. We have diagonalized the Hamiltonian in the subspaces of $r=0,1,3,4$. Now we diagonalize the Hamiltonian in the subspace $r=2$ and use the following notations:

$$\begin{aligned}|1\rangle_1&=|1100\rangle,|n\rangle_1=\mathcal{T}^{n-1}|1\rangle_1(n=1,2,3,4),\\ |1\rangle_2&=|1010\rangle,|m\rangle_2=\mathcal{T}^{m-1}|1\rangle_2(m=1,2).\end{aligned} \tag{13}$$

The action of the Hamiltonian is then described by

$$H|n\rangle_1=2J\sum_{m=1}^{2}|m\rangle_2,H|m\rangle_2=2J\sum_{n=1}^{4}|n\rangle_1. \tag{14}$$

By diagonalizing the corresponding 6×6 matrix the eigenvalues and eigenstates are given by

$$E_{\pm}=\pm 4J\sqrt{2},|\Psi_{\pm}\rangle=\frac{1}{2\sqrt{2}}\left(\sum_{n=1}^{4}|n\rangle_1\pm\sqrt{2}\sum_{m=1}^{2}|m\rangle_2\right),$$

$$E_1=0,|\Psi_1\rangle=\frac{1}{\sqrt{2}}(|1010\rangle-|0101\rangle),$$

$$E_2=0,|\Psi_2\rangle=\frac{1}{\sqrt{2}}(|1100\rangle-|0011\rangle), \tag{15}$$

$$E_3=0,|\Psi_3\rangle=\frac{1}{\sqrt{2}}(|1001\rangle-|0110\rangle),$$

$$E_4=0,|\Psi_4\rangle=\frac{1}{2}(|1100\rangle+|0011\rangle-|1001\rangle-|0110\rangle).$$

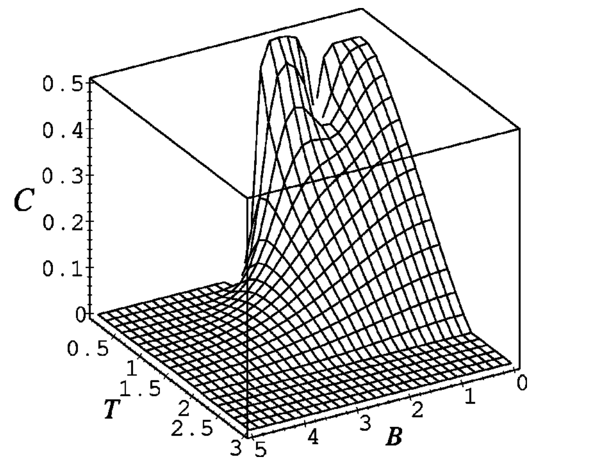

FIG. 1. The concurrence against the temperature and magnetic field. The parameter $J=1$.

From Eqs. (12) and (15) all the eigenvalues are obtained as $\pm 4B$ (1), $\pm 2B$ (2), $4J\pm 2B$ (1), $-4J\pm 2B$ (1), $\pm 4J\sqrt{2}$ (1),0 (4), where the numbers in the parentheses denote the degeneracy. Then the partition function simply follows as

$$\begin{aligned}Z=&4+2\cosh(4\sqrt{2}\beta J)+2\cosh(4\beta B)\\&+4[1+\cosh(4\beta J)]\cosh(2\beta B).\end{aligned} \tag{16}$$

From Eqs. (7), (12), (15), and (16), we get the internal energy, magnetization, and correlation function G_{zz},

$$\begin{aligned}-Z\overline{U}=&2J\sqrt{2}\sinh(4\sqrt{2}\beta J)+2B\sinh(4\beta B)\\&+2B[1+\cosh(4\beta J)]\sinh(2\beta B)\\&+4J\sinh(4\beta J)\cosh(2\beta B),\end{aligned} \tag{17}$$

$$-Z\overline{M}=2\sinh(4\beta B)+2[1+\cosh(4\beta J)]\sinh(2\beta B),$$

$$ZG_{zz}=2\cosh(4\beta B)-\cosh(4\sqrt{2}\beta J)-1.$$

Then according to the relation (6) the correlation function G_{xx} is obtained as

$$G_{xx}Z=-\sqrt{2}\sinh(4\sqrt{2}\beta J)-2\sinh(4\beta J)\cosh(2\beta B). \tag{18}$$

The combination of Eqs. (17), (18), and (5) gives the exact expression of the concurrence. It is easy to see that the concurrence is independent of the sign of J and B, which is consistent with the general result given by Proposition 2 for even-number qubits.

Figure 1 gives a three-dimensional plot of the concurrence against the temperature and magnetic field. The exchange constant J is chosen to be 1 in the following. We observe a threshold temperature $T_c = 2.36338$ after which the entanglement disappears. It is interesting to see that the threshold temperature is independent of the magnetic field B for our four-qubit model. For two-qubit XX model the threshold temperature is also independent of B [3]. We further observe that near the zero temperature there exists a dip when the magnetic field increases from zero. The dip is due to the energy level crossing at point $B_{c1} = 2(\sqrt{2}-1) = 0.82843$. When B increases form $B=2$ near the zero temperature the entanglement disappears quickly since there is another level crossing point $B_{c2}=2$ after which the ground state becomes $|1111\rangle$. We also see that it is possible to increase entanglement by increasing the temperature in the range of magnetic field $B>2$.

Now we discuss the ground-state entanglement ($T=0$). When $B<B_{c1}$, the ground state is $|\Psi_-\rangle$ with the eigenvalue $E^{(0)} = -4\sqrt{2}J$. It is direct to check that $G_{zz}^{(0)} = -1/2$. Then according to Eq. (11), the concurrence is obtained as $C = \sqrt{2}/2 - 1/4 = 0.45711$. When $B_{c1}<B<B_{c2}$ the ground state is $|k=2\rangle'$ and the corresponding concurrence is 1/2. When $B>B_{c2}$ the ground state becomes $|1111\rangle$, so there exists no entanglement.

Thus far we have discussed the *pairwise entanglement* in both the ground state and the thermal state. Now we discuss the many-body entanglement in the ground state. Recently Coffman *et al.* [18] used concurrence to examine three-qubit systems, and introduced the concept of the square 3-bit concurrence as a way to quantify the amount of three way entanglement in three-qubit systems. Later Wong and Christensen [19] generalize the square 3-bit concurrence to the even-number square N-bit concurrence. The square N-bit concurrence is defined as

$$\tau_{1,2,\ldots,N} \equiv |\langle \psi | \sigma_{1y} \otimes \sigma_{2y} \otimes \cdots \otimes \sigma_{Ny} | \psi^* \rangle|^2, \qquad (19)$$

with $|\psi\rangle$ a multiqubit pure state. The square N-bit concurrence works only for an even number of qubits.

For the ground state $|\Psi_-\rangle$ we have $|\Psi_-^*\rangle = |\Psi_-\rangle$, and

$$\sigma_{1y} \otimes \sigma_{2y} \otimes \sigma_{3y} \otimes \sigma_{4y} |\Psi_-\rangle = |\Psi_-\rangle, \qquad (20)$$

i.e., the ground state is an eigenstate of the operator $\sigma_{1y} \otimes \sigma_{2y} \otimes \sigma_{3y} \otimes \sigma_{4y}$. Therefore we find $\tau_{1,2,\ldots,4}=1$, which means that the ground state has four-body maximal entanglement. For another two ground states when varying the magnetic field it is easy to check that $\tau_{1,2,\ldots,4}=0$, which means that the ground states have no genuine four-body entanglement. Note that the ground state $|k=2\rangle'$ has pairwise entanglement, but no four-body entanglement.

In conclusion, we have found that the pairwise thermal entanglement of nearest-neighbor qubits is independent of the sign of exchange constants and the sign of magnetic fields in the XX even-number qubit ring with a magnetic field. For determining the concurrence we need to know not only the partition function, but also one correlation function G_{zz}. For the four-qubit model we observe that there exists a threshold temperature that is independent of the magnetic field. The effects of level crossing on the thermal entanglement and ground-state entanglement are also discussed. Finally we find that the ground state is a four-body maximally entangled state according to the potential many-body entanglement measure, the square N-bit concurrence.

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