Quantum entanglement and Bell inequalities in Heisenberg spin chains

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We show that in one-dimensional isotropic Heisenberg model two-qubit thermal entanglement and maximal violation of Bell inequalities are directly related with a thermodynamical state function, i.e., the internal energy. Therefore they are completely determined by the partition function, the central object of thermodynamics. For ferromagnetic ring we prove that there is no thermal entanglement at any temperature. Explicit relations between the concurrence and the measure of maximal Bell inequality violation are given.

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Over the past few years much effort has been put into studying the entanglement of quantum systems both qualitatively and quantitatively. Entangled states constitute indeed a valuable resource in quantum information processing [1]. Entanglement in systems of interacting spins [2–6] as well as in systems of indistinguishable particles [7–11] has been investigated. In particular entanglement in both the ground state [2,3] and thermal state [4–6] of a spin-1/2 Heisenberg spin chain have been analyzed in the literature. The intriguing issue of the relation between entanglement and quantum phase transition [12] have been addressed in a few quite recent papers [13,14].

From a conceptual perspective one can say that these investigations aim to provide a bridge between quantum information theory and theoretical condensed matter physics. This is done by considering thermal equilibrium in a canonical ensemble. In this situation the system state is given by the Gibb’s density operator \( \rho_T = \exp (-H/kT)/Z \), where \( Z = \text{tr} \{ \exp (-H/kT) \} \) is the partition function, \( H \) the system Hamiltonian, \( k \) is Boltzmann’s constant which we henceforth will take equal to 1, and \( T \) the temperature. As \( \rho(T) \) represents a thermal state, the entanglement in the state is called thermal entanglement [4]. It is important to stress that, although the central object of statistical physics, the partition function, is determined by the eigenvalues of \( H \) only, thermal entanglement properties generally require in addition the knowledge of the energy eigenstates.

On the other hand the violation of Bell inequalities [15] was considered as a means of determining whether there is entanglement. In 1989 Werner [16] demonstrated that there exists states which are entangled but do not violate any Bell-type inequality, i.e., not all entangled states violate a Bell inequality. Further studies [17,18] showed that the maximal violation of a Bell inequality does not behave monotonously under local operation and classical communications. So Bell violations can only be considered an entanglement witness [19]. More recently the relation between Bell inequalities and the usefulness for quantum key distribution and quantum secret sharing have been clarified [20]. Moreover it has been showed that even multipartite bound entangled states can violate Bell inequalities [21].

In this paper we shall study the Heisenberg qubit chains by exploring further connections between entanglement and other relevant physical quantities. We will study the relations between the concurrence, an entanglement measure for two qubits, with thermodynamic potentials such as the internal energy \( U \) and magnetization \( M \). The latter quantities are defined as

\[
U = - \frac{1}{Z} \frac{\partial Z}{\partial B}, \quad M = - \frac{1}{Z} \frac{\partial Z}{\partial \beta},
\]

where \( \beta = 1/T \) and \( B \) is a magnetic field. We shall establish a remarkably simple relation between the concurrence for the thermal state and the internal energy. A direct relation between the maximal violation of the Bell inequality and the internal energy will be given as well.

We first briefly review the definition of concurrence [22]. Let \( \rho_{12} \) be the density matrix of a pair of qubits 1 and 2. The density matrix can be either pure or mixed. The concurrence corresponding to the density matrix is defined as

\[
C = \max \{ \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0 \},
\]

where the quantities \( \lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4 \) are the square roots of the eigenvalues of the operator

\[
\varrho_{12} = \rho_{12} (\sigma_y \otimes \sigma_y) \rho_{12}^* (\sigma_y \otimes \sigma_y).
\]

The nonzero concurrence implies that the qubits 1 and 2 are entangled. The concurrence \( C_{12} = 0 \) corresponds to an unentangled state and \( C_{12} = 1 \) corresponds to a maximally entangled state.

The **Heisenberg model and pairwise entanglement**. We consider a physical model of a chain of \( N \) qubits, namely, a chain of spin-1/2 particles in which neighboring particles interact via the anisotropic Heisenberg Hamiltonian \( H = H(\Delta, B) \), with a magnetic field

\[
H = J \sum_{i=1}^N (\vec{\sigma}_i \cdot \vec{\sigma}_{i+1} + (\Delta - 1)\sigma_{iz}\sigma_{iz+1}) + B \sum_{i=1}^N \sigma_{iz},
\]

where \( \vec{\sigma}_i = (\sigma_{ix}, \sigma_{iy}, \sigma_{iz}) \) is the vector of Pauli matrices and \( J \) is the exchange constants. The positive and negative \( J \) correspond to the antiferromagnetic (AFM) and ferromagnetic (FM) case, respectively.
In particular the isotropic Hamiltonian also commutes
\[ \sum_{\alpha} |\sigma_{\alpha} \rangle \langle \sigma_{\alpha}|, \]
where \( |\sigma_{\alpha} \rangle \) is the spin up (down) state. Another fact is that
\[ [H, S_z] = 0, \]
which guarantees that reduced density matrix \( \rho_{12} \) of two nearest-neighbor qubits, say qubit 1 and 2, for the thermal state has the form [2]
\[
\rho_{12} = \begin{pmatrix}
  u^+ & w_1 & z^* \\
  w_2 & z & u^-
\end{pmatrix}
\]
in the standard basis \( \{ |00\rangle, |01\rangle, |10\rangle, |11\rangle \} \). Here \( S_{\alpha} = \sum_{i=1}^{N} \sigma_\alpha / 2 \) (\( \alpha = x, y, z \)) are the collective spin operators. The reduced density matrix is directly related to various correlation functions \( G_{\alpha \beta} = \langle \sigma_{1\alpha} \sigma_{2\beta} \rangle = \text{tr}(\sigma_{1\alpha} \sigma_{2\beta} \rho_T) \).

Then matrix elements can be written in terms of the correlation functions and the magnetization per site \( M = M/N \) as
\[
\begin{align*}
  u^\pm &= \frac{1}{4} \left( 1 \pm 2M + G_{zz} \right), \\
  z &= \frac{1}{4} \left( G_{xx} + G_{yy} + iG_{xy} - iG_{yx} \right).
\end{align*}
\]

In the deriving of above equation, we have used the translation invariance of the Hamiltonian. From the above equation we find the following relations which will be useful later
\[
\begin{align*}
  u^+ - u^- &= M, \\
  u^+ + u^- &= \frac{1}{2} \left( 1 + G_{zz} \right), \\
  \text{Re}(z) &= \frac{1}{4} (G_{xx} + G_{yy}).
\end{align*}
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All the information needed is contained in the reduced density matrix, from which the concurrence quantifying the entanglement is readily obtained as [2]
\[
C = 2 \max \left[ 0, \left| z - \sqrt{u^+ u^-} \right| \right],
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which can be expressed in terms of the correlation functions and the magnetization as seen from Eq.(6).

Isotropic Heisenberg model. Now we consider the Heisenberg XXX model described by the Hamiltonian
\[ H(1, 0). \]
We first notice that \( H \) admits a continuous \( SU(2) \) group of symmetries. This can be easily checked in that \( H \) commutes with the Lie-algebra generators \( S_{\alpha} \).

In particular the isotropic Hamiltonian also commutes with the operators
\[
Q_{\alpha} = \sigma_{\alpha} \otimes N \quad (\alpha = x, y, z)
\]
that generate \( Z_2 \) sub-groups of \( SU(2) \). The rich rotational symmetry structure of the XXX model along with translational invariance will play a key role in our study of the ring entanglement.

Form the \( Z_2 \) symmetry immediately follows

**Proposition 1.** For any temperature the magnetization \( M \) is vanishing and the nondiagonal element \( z \) is real.

In order to enact translational invariance for finite \( N \) we assume periodic boundary conditions, i.e., \( N + 1 \equiv 1 \), turning the chain into a ring. Therefore \( H \) becomes invariant under cyclic shifts generated by the right shift operator \( T \). The latter being defined by its action on the product basis, \( T |m_1, \ldots, m_{N-1}, m_N \rangle = |m_N, \ldots, m_1, m_{N-1} \rangle \), where \( m_i = 0 \) (1) represents the state of spin up (down). Another fact is that
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Form the \( Z_2 \) symmetry immediately follows

**Proposition 1.** For any temperature the magnetization \( M \) is vanishing and the nondiagonal element \( z \) is real.
Theorem 1 The concurrence of the nearest-neighbor qubits in the Heisenberg model is given by

$$C = \begin{cases} \frac{1}{2} \max[0, -\frac{u}{\beta JN}] - 1 & \text{for AFM,} \\ \frac{1}{2} \max[0, \frac{3U}{3JN}] - 1 & \text{for FM.} \end{cases} \tag{12}$$

In the limit $T \to 0$ in the antiferromagnetic even-site model, the thermal state becomes the nondegenerate ground state. As we expected Eq.(12) reduces to Eq.(11) in this limit. Theorem 1 establishes a direct relation between the concurrence and a macroscopic thermodynamical function, the internal energy. Then the entanglement is uniquely determined by the partition function of the system. Notice that Theorem 1 has no restriction to even or odd number of qubits.

**Corollary 1** At any temperature there is no thermal entanglement between two qubits in the FM XXX Heisenberg rings.

Now we discuss the case of AFM. When the temperature increases the internal energy will increase but the concurrence decreases. When the internal energy arrives at $-NJ$ the concurrence becomes zero.

The temperature $T_c$ at which the concurrence vanishes is called the threshold temperature. In a short summary we have

**Corollary 2** At temperatures lower than $T_c$ there exists thermal entanglement between two qubits in the AFM XXX Heisenberg rings. $T_c$ is determined by the equation $u(N) = U(T_c)/(\beta JN) = 1$. From the numerical evidences of Refs. [2] and [23] we conjecture that $u(N)$ is a non-increasing (non-decreasing) function of $N$ for $N$ even (odd). Therefore since it has been estimated $u(\infty) > 1$ [2] and $u(3) < 1$ [23] one obtains that the ground state of the AFM Heisenberg is always entangled except for the case $N = 3$.

Now we give the examples of 2 and 3 qubit for the illustration of our general results. For two-qubit model the partition function is given by $Z = 3e^{-2\beta J} + e^{3\beta J}$, then the internal energy follows $6J(e^{-2\beta J} - e^{3\beta J})/Z$. From Eq.(12) the concurrence is found to be zero for the FM rings and $C = \max[0, \exp(8\beta J) - 3]/\exp(8\beta J) + 3]$ for the AFM [4]. The threshold temperature is then determined by $\exp(8\beta J) = 3$ and it is given by $T_c = 8J/\ln 3$. For three-qubit model the partition function is given by $8\cosh(3\beta J)$, and then the internal energy is

$$-3J \tanh(3\beta J),$$

from which and Eq.(12) we can find that the concurrence is zero for the FM rings as we expected and $C = \max[0, \tanh(3\beta J) - 1]/2$. Hence we recover the result that there is no pairwise thermal entanglement for the three-qubit Heisenberg ring [6]. Next we discuss Bell inequality.

**Bell inequality.** The most commonly discussed Bell-inequality is the CHSH inequality [15,24]. The CHSH operator $(\vec{a}, \vec{a}^\prime, \vec{b}, \vec{b}^\prime$ are unit vectors) reads

$$B = \vec{a} \cdot \vec{\sigma} \otimes (\vec{b} + \vec{b}^\prime) \cdot \vec{\sigma} + \vec{a}^\prime \cdot \vec{\sigma} \otimes (\vec{b} - \vec{b}^\prime) \cdot \vec{\sigma}. \tag{14}$$

In the above notation, the Bell inequality reads

$$|\langle B \rangle| = |\text{tr}(\rho B)| \leq 2, \tag{15}$$

where $\rho$ is an arbitrary two-qubit state. The maximal amount of Bell violation of a state $\rho$ is given by [25]

$$B = 2\sqrt{u} + \tilde{u}, \tag{16}$$

where $u$ and $\tilde{u}$ are the two largest eigenvalues of $T_\rho T_\rho^\dagger$. The matrix $T_\rho$ is determined completely by the correlation functions being a $3 \times 3$ matrix whose elements are $(T_\rho)_{nm} = \text{tr}(\rho_{02}\sigma_n \otimes \sigma_m)$. Here $\sigma_x \equiv \sigma_z, \sigma_y \equiv \sigma_y$, and $\sigma_3 \equiv \sigma_z$ are the usual Pauli matrices. We call the quantity $B$ the maximal violation measure, which indicates the Bell violation when $B > 2$ and the maximal violation when $B = 2\sqrt{2}$. The violation measure is a function of the correlation functions and does not depend on the magnetization.

For the isotropic Heisenberg model the matrix $T_\rho$ is easily obtained as $\text{diag}[G_{xx}, G_{xx}, G_{xx}]$ and the violation measure becomes

$$B = 2\sqrt{2}G_{xx} = \frac{-2\sqrt{2}}{2\sqrt{2}} \frac{3\beta J}{3N} \text{ For AFM,}$$

$$\frac{2\sqrt{2}}{3\beta J} \text{ For FM.} \tag{17}$$

As we expected, the violation measure is completely determined by the internal energy just as the concurrence.

From Eqs.(12) and (17) we arrive at an explicit relation between the concurrence and the violation measure

$$C = \begin{cases} \frac{1}{2} \max[0, \frac{3\beta J}{3N}] - 1 & \text{For AFM,} \\ \frac{1}{2} \max[0, \frac{3\beta J}{2\sqrt{2}}] - 1 & \text{For FM.} \end{cases} \tag{18}$$

From the above relation we know that the concurrence is larger than zero when the Bell inequality is violated. When $2\sqrt{2}/3 < B \leq 2$ for the AFM rings the state is entangled, but the Bell inequality is not violated. The result is general for arbitrary $N$. The maximal value of $B$ is $2\sqrt{2}$, therefore the concurrence is zero for the FM rings. Next we consider the general model with anisotropy and magnetic fields.

**General models including anisotropy and magnetic fields.** For $\Delta \neq 1$ one obtains an anisotropic model which has no longer a global SU(2)-symmetry. The corresponding Hamiltonian $H(\Delta, 0)$ still commutes with the $z$ component of the total spin. So the concurrence is given by...
Eq. (9). For this model we have the following relations
\[ \bar{U}/J = G'_{xx} + G'_{yy} + \Delta G_{zz} \],
where \( \bar{U} = U/N \) is the internal energy per site. The combination of the relation and
Eq. (9) gives
\[ C = \frac{1}{2} \max[0, |\bar{U}/J - \Delta G_{zz} - G_{zz} - 1|]. \] (19)

Then if we calculate the concurrence, we need to know the correlation function \( G_{zz} \), and the partition function.
The partition function itself is not sufficient for determining the entanglement. In particular for \( XY \) model, i.e.,
\( \Delta = 0 \), the concurrence reduces to
\[ C = \frac{1}{2} \max[0, |\bar{U}/J - G_{zz} - 1|]. \]
We still need to know the correlation function \( G_{zz} \) [26] to calculate the concurrence.

Now we consider the \( XXX \) model with a magnetic field, i.e., the Hamiltonian \( H(1, B) \). Now the magnetization
is not long zero and hence \( u^+ \neq u^- \). For this model we have the relation
\[ \bar{U}/J = G_{xx} + G_{yy} + G_{zz} + BM = 4 \text{Re}(z) + 2(u^+ - u^-) + 1 + BM. \]
Here we have used the relation
\[ \alpha \bar{g} = N(1 - BM)^2 - 2M^2 \sqrt{1/2}. \] To calculate the entanglement we need to know, beside
the threshold temperature), no pairwise thermal entanglement for the thermal states.

\( \bar{G}_{zz} \) is the internal energy. This result is noteworthy and somewhat
The key ingredient in our derivations has been the vast symmetry group of the
Heisenberg qubit rings. In the isotropic case we found
of the thermal state is given, with an extra \( \alpha \), dependence, by Eq. (9). If
\[ J_{i,j}^x = J_{i,j}^y = J_{i,j}^z \] then it is easy to check that the Hamiltonian \( H \) has a global
\( SU(2) \)-symmetry. Therefore the concurrence becomes
\[ C = \frac{1}{2} \max[0, 2|G_{zz} - G_{zz} - 1|], \]
which is determined solely by the correlation function \( G_{zz} \).

Comments. Our discussions above are applicable to more general Heisenberg Hamiltonians such as
\[ \sum_{i \neq j} (J_{i,j}^x \sigma_i^x \sigma_j^x + J_{i,j}^y \sigma_i^y \sigma_j^y + J_{i,j}^z \sigma_i^z \sigma_j^z), \] (20)
where \( J_{i,j}^\alpha (\alpha = x, y, z) \) are arbitrary exchange constants.
For this model we still have the \( Z_2 \) symmetry \( [H, \sigma^N_z] = 0 \). Therefore the concurrence for the two qubits \( i \) and
\( j \) of the thermal state is given, with an extra \( \i, j \) dependence, by Eq. (9). If
\( J_{i,j}^x = J_{i,j}^y = J_{i,j}^z \) then it is easy to check that the Hamiltonian \( H \) has a global
\( SU(2) \)-symmetry. Therefore the concurrence becomes
\[ C = \frac{1}{2} \max[0, 2|G_{zz} - G_{zz} - 1|], \]
which is determined solely by the correlation function \( G_{zz} \).

Conclusions. In this paper we have discussed thermal entanglement and Bell inequality violation in the
Heisenberg qubit rings. In the isotropic case we found that there exists a simple relation between the pairwise
entanglement for the thermal states and the internal energy. This result is noteworthy and somewhat
surprising in that it allows to directly connect entanglement properties with a thermodynamical potential and
thus eventually with the partition function. In particular one can conclude that, at any temperature (above
the threshold temperature), no pairwise thermal entanglement exists in the FM (AFM) rings.
We also determined a simple relation between the measure of maximal violation of Bell inequality and the
internal energy. This in turn allows to explicitly show the relation between the concurrence and the violation
measure. The key ingredient in our derivations has been the vast symmetry group of the \( XXX \) model. The study of
the relation between thermal entanglement and thermodynamical quantities for spin models with a poorer
symmetry structure is, we believe, an intriguing challenge for future investigations.

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