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How to cite:

Fu, Hongchen; Solomon, Allan I. and Wang, Xiaoguang (2003). Critical temperature for entanglement transition in Heisenberg models. In: Group 24; Physical and Mathematical Aspects of Symmetries, 2003.

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Critical temperature for entanglement transition in Heisenberg Models

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Abstract. We study thermal entanglement in some low-dimensional Heisenberg models. It is found that in each model there is a critical temperature above which thermal entanglement is absent.

1. Introduction

Entanglement[1] plays an important role in quantum computation and quantum information processing. With appropriate coding, a system of interacting spins, such as described by a Heisenberg hamiltonian, can be used to model a solid-state quantum computer. It is therefore of some significance to study thermal entanglement in Heisenberg models. We find that for each model there is a corresponding critical temperature for transition to the entanglement regime, and the entanglement only occurs below this critical temperature.

2. Measures of entanglement

A pure state described by the wave function $|\Psi\rangle$ is *non-entangled* if it can be factorized as $|\Psi\rangle = |\Psi_1\rangle \otimes |\Psi_2\rangle$. Otherwise, it is entangled. A typical example of an entangled state is the Bell state for a bipartite system of two qubits:

$$\frac{1}{\sqrt{2}}(|01\rangle - |10\rangle) \tag{1}$$

For such a bipartite system the most popular entanglement measure is the *entanglement of formation*. For a pure state the entanglement of formation is defined as the reduced entropy of either subsystem[2].

For the two-qubit system one can use *concurrence*[3] as a measure of the entanglement. Let ρ_{12} be the density matrix of the pair which may represent either a pure or a mixed state. The concurrence corresponding to the density matrix is defined as

$$\mathcal{C}_{12} = \max\left\{\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0\right\},\tag{2}$$

where the quantities λ_i are the square roots of the eigenvalues of the operator

$$\varrho_{12} = \rho_{12}(\sigma_1^y \otimes \sigma_2^y)\rho_{12}^*(\sigma_1^y \otimes \sigma_2^y) \tag{3}$$

in descending order. The eigenvalues of ρ_{12} are real and non-negative even though ρ_{12} is not necessarily Hermitian. The entanglement of formation is a monotonic function of the concurrence, whose values range from zero, for an non-entangled state, to one, for a maximally entangled state.

3. Heisenberg models

The general N-qubit Heisenberg XYZ model in a magnetic field B is described by the Hamiltonian

$$H = \frac{1}{2} \sum_{n=1}^{N} \left(\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + \sigma_n^z \sigma_{n+1}^z \right) + \sum_{n=1}^{N} B_n \sigma_n^z \tag{4}$$

where we assume cyclic boundary conditions $N + 1 \equiv 1$. The Gibbs state of a system in thermodynamic equilibrium is represented by the density operator

$$\rho(T) = \exp(-H/kT)/Z,\tag{5}$$

where Z = tr[exp(-H/kT)] is the partition function, k is Boltzmann's constant which we henceforth take equal to 1, and T is the temperature.

As $\rho(T)$ represents a thermal state, the entanglement in the state is called *thermal* entanglement. At T = 0, $\rho(0)$ represents the ground state which is pure for the non-degenerate case and mixed for the degenerate case. The ground state may be entangled. At $T = \infty$, $\rho(\infty)$ is a completely random mixture and cannot be entangled.

4. Thermal entanglement in the 2-site Heisenberg model

The density matrix can be obtained [4] as

$$\rho(T) = A \begin{pmatrix} e^{-B/T} & \\ & \cosh(J/T) & -\sinh(J/T) & \\ & -\sinh(J/T) & \cosh(J/T) & \\ & & e^{B/T} \end{pmatrix}$$
(6)

where $A = (2\cosh(J/T) + 2\cosh(B/T))^{-1}$, and the concurrence

$$C = \max\left\{\frac{\sinh(J/T) - 1}{\cosh(J/T) + \cosh(B/T)}, 0\right\}.$$
(7)

As the denominator is always positive, the entanglement condition is

$$\sinh(J/T) - 1 > 0$$
 or $T < 1.134J.$ (8)

from which we conclude that

- There is a critical temperature $T_c \sim 1.134 J$. The thermal state is entangled when $T < T_c$.
- The critical temperature is independent of the magnetic field *B*.
- Entanglement occurs only for the antiferromagnetic case (J > 0).

5. Thermal entanglement in the 3-site Heisenberg model

We now consider pairwise entanglement in the 3-site Heisenberg model with uniform magnetic field, and also in the presence of a magnetic impurity[5]. The reduced density matrix of two sites can be written as

$$\rho_{12} = \frac{2}{3Z} \begin{pmatrix} u & & \\ & w & y & \\ & y & w & \\ & & & v \end{pmatrix}$$
(9)

The concurrence may be readily obtained as

$$C = \frac{4}{3Z} \max\{|y| - \sqrt{uv}, 0\},$$
(10)

In the case of a uniform magnetic field, the entanglement between any two sites is the same due to cyclic symmetry. We therefore need only consider the entanglement between sites 1 and 2. Then

$$u(B) = v(-B) = \frac{3}{2}e^{3\beta B} + \frac{1}{2}e^{\beta B}(2z + z^{-2})$$

$$w = \cosh(\beta B)(2z + z^{-2})$$

$$y = \cosh(\beta B)(z^{-2} - z)$$

$$Z = 2\cosh(3\beta B) + 2\cosh(\beta B)(2z + z^{-2}).$$
 (11)

where $(z = \exp(\beta J))$.

If B = 0, one can easily find that the sites 1 and 2 are entangled if and only if

$$2|z^{-2} - z| - 3 - 2z - z^{-2} > 0 \tag{12}$$

from which we conclude that

- There is no entanglement when J > 0;
- Entanglement occurs when J < 0 and $T < T_c$, where the critical temperature is given by -1.27J = 1.27|J|.
- The maximal concurrence is 1/3, which occurs for $T \to 0$.

Fig.1 plots the concurrence against τ for different *B*. From these graphs we see that there exists a critical temperature above which the entanglement vanishes. It is also noteworthy that the critical temperature increases as the magnetic field *B* increases.

We now consider the case of a single impurity field on the third site; thus $B_1 = B_2 = 0$ and $B_3 = BJ > 0$. In this case the cyclic symmetry is violated and we have to consider the entanglement between sites 1 and 2, and between sites 1 and 3, separately.

Fig.2 plots the concurrence C_{12} and C_{13} against scaled temperature $\tau = kt/|J|$ for different magnetic fields *B*. From Fig.2(a) we see that when the magnetic field is located at the third site both the antiferromagnetic and ferromagnetic cases are entangled in the range $0 < \tau \leq \tau_c$, where the critical temperature τ_c depends on *B*. Fig.2(a) also suggests that the concurrence C_{12} tends to 1, namely that the (1,2) entanglement becomes maximal, when $\tau \to 0$ for large enough *B*, in both the antiferromagnetic cases.

In contrast to the (1, 2) case, the entanglement between sites 1 and 3 increases to a maximum with increasing B and then decreases. The lower the τ , the smaller the



Figure 1. Concurrence as a function of T for different magnetic fields B = 1(solid line), 3/2(dashed line), and 2(circle point line).



Figure 2. Concurrence C_{12} C_{13} against τ for different *B*. For antiferromagnetic case (dotted line), B = 10.

B at which the concurrence reaches its maximum value. For smaller B, entanglement occurs only in the ferromagnetic case (J < 0), while for large enough B (e.g. B = 10 in our units), weak entanglement occurs in both the antiferromagnetic and ferromagnetic cases.

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