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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:

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

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  $\rho_{12}$  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

$$C_{12} = \max \{ \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0 \}, \quad (2)$$

where the quantities  $\lambda_i$  are the square roots of the eigenvalues of the operator

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

in descending order. The eigenvalues of  $\varrho_{12}$  are real and non-negative even though  $\varrho_{12}$  is not necessarily Hermitian. The entanglement of formation is a monotonic function of the concurrence, whose values range from zero, for a 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

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

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

$$\rho(T) = \exp(-H/kT)/Z, \quad (5)$$

where  $Z = \text{tr}[\exp(-H/kT)]$  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

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

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

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

As the denominator is always positive, the entanglement condition is

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

from which we conclude that

- There is a critical temperature  $T_c \sim 1.134J$ . 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

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

The concurrence may be readily obtained as

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

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

$$\begin{aligned} u(B) &= v(-B) = \frac{3}{2}e^{3\beta B} + \frac{1}{2}e^{\beta B}(2z + z^{-2}) \\ w &= \cosh(\beta B)(2z + z^{-2}) \\ y &= \cosh(\beta B)(z^{-2} - z) \\ Z &= 2 \cosh(3\beta B) + 2 \cosh(\beta B)(2z + z^{-2}). \end{aligned} \quad (11)$$

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

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

$$2|z^{-2} - z| - 3 - 2z - z^{-2} > 0 \quad (12)$$

from which we conclude that

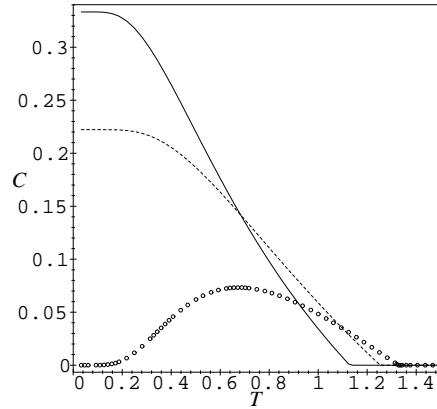
- There is no entanglement when  $J > 0$ ;
- Entanglement occurs when  $J < 0$  and  $T < T_c$ , where the critical temperature is given by  $-1.27J = 1.27|J|$ .
- The maximal concurrence is  $1/3$ , which occurs for  $T \rightarrow 0$ .

Fig.1 plots the concurrence against  $\tau$  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.

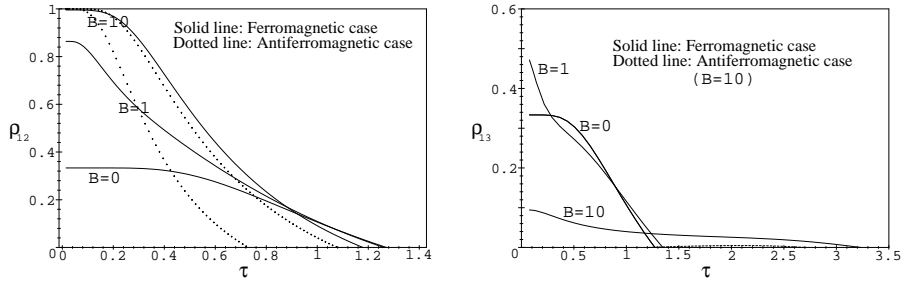
We now consider the case of a single impurity field on the third site; thus  $B_1 = B_2 = 0$  and  $B_3 = BJ > 0$ . In this case the cyclic symmetry is violated and we have to consider the entanglement between sites 1 and 2, and between sites 1 and 3, separately.

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  $\tau_c$  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  $\tau \rightarrow 0$  for large enough  $B$ , in both the antiferromagnetic and ferromagnetic 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  $\tau$ , 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  $\tau$  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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