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

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

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

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

As the denominator is always positive, the entanglement condition is

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

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

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

The concurrence may be readily obtained as

$$C = \frac{4}{3Z}\max\left\{|y| - \sqrt{uv}, 0\right\}, \tag{10}$$

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

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

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 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 τ, the smaller the

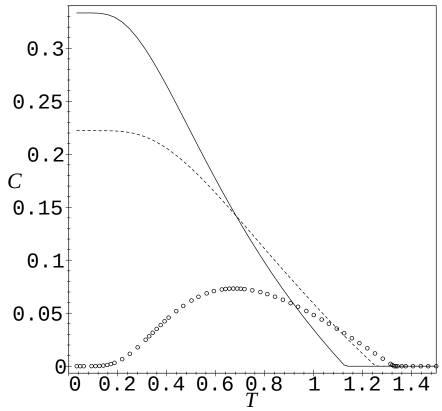

Figure 1. Concurrence as a function of T for different magnetic fields $B = 1$(solid line), 3/2(dashed line), and 2(circle point line).

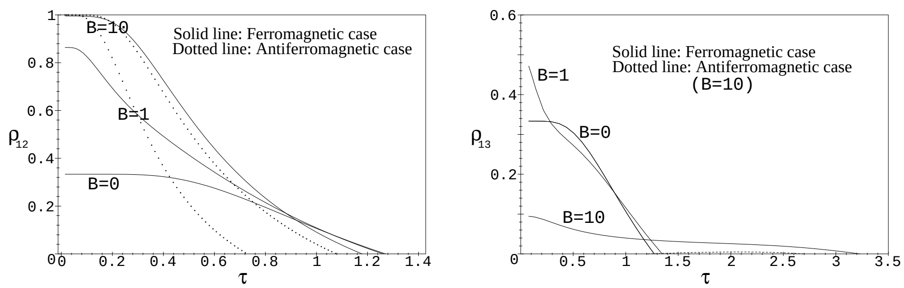

Figure 2. Concurrence C_{12} C_{13}against τ for different B. For antiferromagnetic case (dotted line), $B = 10$.

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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