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Pairwise entanglement in the *XX* model with a magnetic impurity

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Abstract

For a three-qubit Heisenberg model in a uniform magnetic field, the pairwise thermal entanglement of any two sites is identical due to the *exchange* symmetry of sites. In this paper we consider the effect of a non-uniform magnetic field on the Heisenberg model, modelling a magnetic impurity on one site. Since pairwise entanglement is calculated by tracing out one of the three sites, the entanglement clearly depends on which site the impurity is located. When the impurity is located on the site which is traced out, that is, when it acts as an *external field* of the pair, the entanglement can be enhanced to the maximal value 1; while when the field acts on a site of the pair the corresponding concurrence can only be increased from $1/3$ to $2/3$.

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1. Introduction

There is currently an ongoing effort to study entanglement in multipartite systems, since such entangled states may provide a valuable resource in quantum information processing [1]. Recently entanglements in quantum operations [2–4] and in indistinguishable fermionic and bosonic systems [5–7] have been considered. Entanglement in two-qubit states has been well studied in the literature. Various kinds of three-qubit entangled states have also been studied [8–10], which have been shown to possess advantages over two-qubit states in quantum teleportation [11], dense coding [12] and quantum cloning [13].

One interesting and natural type of entanglement, thermal entanglement, was introduced and studied in the context of the Heisenberg *XXX* [14], *XX* [15], and *XXZ* [16] models as well as the Ising model in a magnetic field [17]. The Heisenberg interaction has been used to simulate a quantum computer [18], and can also be realized in quantum dots [18], nuclear spins [19], electronic spins [20] and optical lattices [21]. By suitable coding, the Heisenberg

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interaction can be used for quantum computation [22]. Entanglement in the ground state of the Heisenberg model has been discussed previously [23]. In an earlier note [24] we presented an analytical study of pairwise entanglement in the three-qubit Heisenberg model in a *uniform* magnetic field and found that the magnetic field can greatly enhance pairwise entanglement. Due to *exchange* symmetry in this cyclic model the entanglement of any two sites is identical.

In this paper we consider the effect of a magnetic impurity on entanglement in the Heisenberg model. We find unsurprisingly that the effect of such an inhomogeneous magnetic field on the entanglement depends on which site the impurity is located, although in a non-intuitive way. When the field may be considered as an *external field* of the pair, that is, when it is located on the site which is traced over, then it can enhance the entanglement to its maximal value, as measured by the concurrence. When the field acts on a site of the pair the concurrence can be increased from 1/3 to 2/3, but not to its maximal value 1.

2. *XX* Heisenberg model with magnetic impurity

We consider the three-qubit *XX* Heisenberg model in a magnetic field acting on the third site only. The Hamiltonian is [25]

$$H = \frac{J}{2}\sum_{i=1}^{3}\left(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y\right) + BJ\sigma_3^z \tag{1}$$

where we use BJ rather than B to denote the magnetic field. The Hamiltonian (1) has eight distinct eigenvalues when $B \neq 0$

$$\begin{aligned} E_0 &= -JB & E_1 &= \frac{J}{2}(1+B_-) \\ E_2 &= -J(1+B) & E_3 &= -J(1-B) \\ E_4 &= \frac{J}{2}(1+B_+) & E_5 &= \frac{J}{2}(1-B_-) \\ E_6 &= \frac{J}{2}(1-B_+) & E_7 &= JB \end{aligned} \tag{2}$$

where $B_\pm \equiv (4B^2 \pm 4B + 9)^{1/2}$. When $B = 0$, the energy levels are degenerate

$$E_1 = E_7 = 0 \qquad E_1 = E_3 = E_4 = 2J \qquad E_2 = E_5 = E_6 = -J. \tag{3}$$

In the antiferromagnetic case ($J > 0$), the ground state is E_2, while in the ferromagnetic case ($J < 0$), the ground state is E_4.

The corresponding non-degenerate, orthogonal eigenstates are

$$\begin{aligned} |\phi_0\rangle &= |000\rangle \\ |\phi_1\rangle &= \mathcal{N}_1\left(|100\rangle + |010\rangle + a_1|001\rangle\right) \\ |\phi_2\rangle &= 2^{-1/2}\left(|010\rangle - |100\rangle\right) \\ |\phi_3\rangle &= 2^{-1/2}\left(|101\rangle - |011\rangle\right) \\ |\phi_4\rangle &= \mathcal{N}_4\left(a_4|110\rangle + |101\rangle + |011\rangle\right) \\ |\phi_5\rangle &= \mathcal{N}_5\left(|100\rangle + |010\rangle + a_5|001\rangle\right) \\ |\phi_6\rangle &= \mathcal{N}_6\left(a_6|110\rangle + |101\rangle + |011\rangle\right) \\ |\phi_7\rangle &= |111\rangle \end{aligned} \tag{4}$$

where

$$\begin{aligned} a_1 &= -\tfrac{1}{2} + \tfrac{1}{2}B_- + B & a_5 &= -\tfrac{1}{2} - \tfrac{1}{2}B_- + B \\ a_4 &= -\tfrac{1}{2} + \tfrac{1}{2}B_+ - B & a_6 &= -\tfrac{1}{2} - \tfrac{1}{2}B_+ - B \end{aligned} \tag{5}$$

and $\mathcal{N}_i = \left(2 + a_i^2\right)^{-1/2}$ ($i = 1, 4, 5, 6$) are normalization constants.

It is interesting to note that the eigenvalues transform under $B \leftrightarrow -B$ by

$$E_0 \leftrightarrow E_7 \qquad E_1 \leftrightarrow E_4 \qquad E_2 \leftrightarrow E_3 \qquad E_5 \leftrightarrow E_6 \tag{6}$$

and so the a_i transform by $a_1 \leftrightarrow a_4, a_5 \leftrightarrow a_6$. This leads to invariance of the entanglement under $B \leftrightarrow -B$.

The density operator $\rho(T)$ at temperature T can be written as

$$\rho(T) = \frac{1}{Z}\sum_{i=0}^{7} \mathrm{e}^{-\beta E_i} |\phi_i\rangle\langle\phi_i| \tag{7}$$

where $\beta = 1/kT$ and Z is the partition function

$$Z = \mathrm{tr}(\mathrm{e}^{-\beta H}) = \sum_{i=0}^{7} \mathrm{e}^{-\beta E_i} \tag{8}$$

$$= 2(1+\mathrm{e}^{J\beta})\cosh(J\beta B) + 2\,\mathrm{e}^{-J\beta/2}\left[\cosh\left(\tfrac{1}{2}J\beta B_+\right) + \cosh\left(\tfrac{1}{2}J\beta B_-\right)\right]. \tag{9}$$

3. Concurrence of pairwise entanglement

The easiest way to calculate the entanglement is by means of the *concurrence* $\mathcal{C}$ [26] between a pair of qubits, which is defined as

$$\mathcal{C} = \max\{\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0\} \tag{10}$$

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

$$\varrho = \rho\left(\sigma_1^y \otimes \sigma_2^y\right)\rho^*\left(\sigma_1^y \otimes \sigma_2^y\right) \tag{11}$$

in descending order; ρ is the density operator of the pair and it can be either pure or mixed. The entanglement of formation is a monotonic function of the concurrence $\mathcal{C}$, varying between a minimum of zero for $\mathcal{C} = 0$, and a maximum of 1 for $\mathcal{C} = 1$.

We now derive the concurrence for any pair of sites in our model. Due to symmetry under the exchange of sites 1 and 2, the entanglement between sites 1 and 3 is the same as that between sites 2 and 3, and so we need only consider entanglement between sites 1 and 3, and between sites 1 and 2.

Taking the trace over the second (third) site, we can obtain the reduced density operator ρ_{13} (ρ_{12}) of the sites 1 and 3 (1 and 2). Both ρ_{12} and ρ_{13} take the following form:

$$\rho = \frac{1}{Z}\begin{pmatrix} u & & & \\ & w_1 & y & \\ & y & w_2 & \\ & & & v \end{pmatrix}. \tag{12}$$

Here, for ρ_{12}, the nonzero matrix elements are given by

$$\begin{aligned} y &= \mathcal{N}_1^2\,\mathrm{e}^{-\beta E_1} + \mathcal{N}_4^2\,\mathrm{e}^{-\beta E_4} + \mathcal{N}_5^2\,\mathrm{e}^{-\beta E_5} + \mathcal{N}_6^2\,\mathrm{e}^{-\beta E_6} - \tfrac{1}{2}\,\mathrm{e}^{-\beta E_2} - \tfrac{1}{2}\,\mathrm{e}^{-\beta E_3} \\ w_1 = w_2 &= \mathcal{N}_1^2\,\mathrm{e}^{-\beta E_1} + \mathcal{N}_4^2\,\mathrm{e}^{-\beta E_4} + \mathcal{N}_5^2\,\mathrm{e}^{-\beta E_5} + \mathcal{N}_6^2\,\mathrm{e}^{-\beta E_6} + \tfrac{1}{2}\,\mathrm{e}^{-\beta E_2} + \tfrac{1}{2}\,\mathrm{e}^{-\beta E_3} \\ u &= \mathrm{e}^{-\beta E_0} + a_1^2\mathcal{N}_1^2\,\mathrm{e}^{-\beta E_1} + a_5^2\mathcal{N}_5^2\,\mathrm{e}^{-\beta E_5} \\ v &= \mathrm{e}^{-\beta E_7} + a_4^2\mathcal{N}_4^2\,\mathrm{e}^{-\beta E_4} + a_6^2\mathcal{N}_6^2\,\mathrm{e}^{-\beta E_6}. \end{aligned} \tag{13}$$

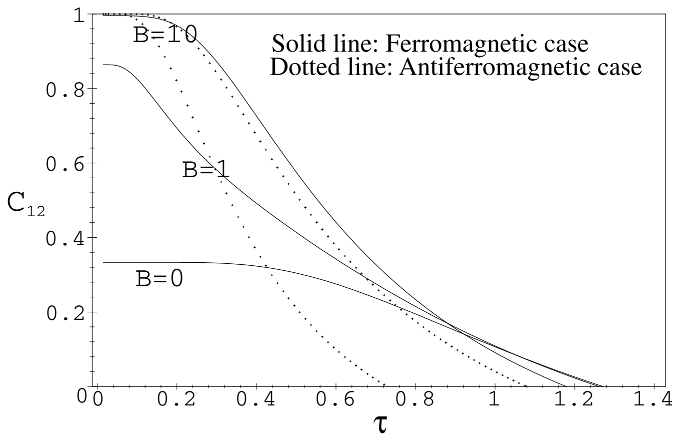

Figure 1. Concurrence $\mathcal{C}_{12}$ against τ for different magnetic fields $B = 0, 1, 10$.

while for the ρ_{13} case, we have

$$\begin{aligned}
y &= a_1\mathcal{N}_1^2\,\mathrm{e}^{-\beta E_1} + a_4\mathcal{N}_4^2\,\mathrm{e}^{-\beta E_4} + a_5\mathcal{N}_5^2\,\mathrm{e}^{-\beta E_5} + a_6\mathcal{N}_6^2\,\mathrm{e}^{-\beta E_6}\\
w_1 &= a_1^2\mathcal{N}_1^2\,\mathrm{e}^{-\beta E_1} + \tfrac{1}{2}\,\mathrm{e}^{-\beta E_3} + \mathcal{N}_4^2\,\mathrm{e}^{-\beta E_4} + a_5^2\mathcal{N}_5^2\,\mathrm{e}^{-\beta E_5} + \mathcal{N}_6^2\,\mathrm{e}^{-\beta E_6}\\
w_2 &= \mathcal{N}_1^2\,\mathrm{e}^{-\beta E_1} + \tfrac{1}{2}\,\mathrm{e}^{-\beta E_2} + a_4^2\mathcal{N}_4^2\,\mathrm{e}^{-\beta E_4} + \mathcal{N}_5^2\,\mathrm{e}^{-\beta E_5} + a_6^2\mathcal{N}_6^2\,\mathrm{e}^{-\beta E_6}\\
u &= \mathrm{e}^{-\beta E_0} + \mathcal{N}_1^2\,\mathrm{e}^{-\beta E_1} + \tfrac{1}{2}\,\mathrm{e}^{-\beta E_2} + \mathcal{N}_5^2\,\mathrm{e}^{-\beta E_5}\\
v &= \mathrm{e}^{-\beta E_7} + \tfrac{1}{2}\,\mathrm{e}^{-\beta E_3} + \mathcal{N}_4^2\,\mathrm{e}^{-\beta E_4} + \mathcal{N}_6^2\,\mathrm{e}^{-\beta E_6}.
\end{aligned} \tag{14}$$

The concurrence has the form

$$\mathcal{C} = \frac{2}{Z}\max\{|y| - \sqrt{uv}, 0\}. \tag{15}$$

The system is entangled when $\mathcal{C} > 0$, and maximally entangled when $\mathcal{C} = 1$. The exchange interaction constant J and the temperature T always appear in the form J/kT in the concurrence and thus we can define the *scaled temperature* $\tau \equiv kT/|J| \geqslant 0$. The concurrence is a function of τ and B.

From equations (6) it is easy to see that $y \to y$ and $u \leftrightarrow v$ when $B \to -B$. This means that the concurrence is invariant under $B \leftrightarrow -B$;

$$\mathcal{C}(\tau, B) = \mathcal{C}(\tau, -B). \tag{16}$$

We therefore only consider the case $B \geqslant 0$ case hereafter.

4. Discussion and results

4.1. $\mathcal{C}_{12}$

We first consider the entanglement between sites 1 and 2. In figures 1 and 2 we give plots of the concurrence of ρ_{12} against τ and B. We know that the entanglement appears only in the antiferromagnetic case ($0 < \tau \leqslant 1.27$) when $B = 0$ [24] (also see figure 1). From figures 1 and 2 we see that, when the magnetic impurity is located at the third site, both the antiferromagnetic and ferromagnetic cases are entangled in the range $0 < \tau \leqslant \tau_0$, where τ_0 depends on B.

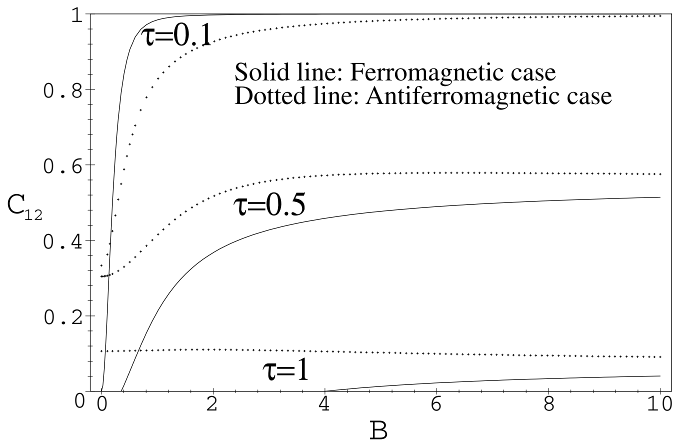

Figure 2. Concurrence $\mathcal{C}_{12}$ against B at different temperatures $\tau = 0.1$, 0.5 and 1.

Figure 1 also suggests that the concurrence $\mathcal{C}_{12}$ goes to 1, namely, the sites 1 and 2 reach maximal entanglement, when $\tau \to 0$ for large enough B, in both the antiferromagnetic and ferromagnetic cases. This fact can be shown analytically as follows.

Consider first the antiferromagnetic case ($J > 0$). In this case E_2 is the ground state; that is, $E_2 - E_i < 0$ for all $i \neq 2$ and thus $\mathrm{e}^{-\beta E_2} \gg \mathrm{e}^{-\beta E_i}$ for $i \neq 2$ in the limit $\tau \to 0$. Note that all $\mathcal{N}_i$ and a_i are finite. Then we have

$$y \to \frac{1}{2}\,\mathrm{e}^{-\beta E_2} \qquad Z \to \mathrm{e}^{-\beta E_2} \qquad \frac{u}{Z} \to 0 \qquad \frac{v}{Z} \to 0 \tag{17}$$

namely, $\mathcal{C}_{12} \to 1$ when $\tau \to 0$.

For the ferromagnetic case ($J < 0$), one can check that $E_4 - E_i < 0$ for all $i \neq 4$ and $\mathrm{e}^{-\beta E_4} \gg \mathrm{e}^{-\beta E_i}$ ($i \neq 4$) in the limit $\tau \to 0$. Then we have

$$y \to \mathcal{N}_4^2\,\mathrm{e}^{-\beta E_4} \qquad Z \to \mathrm{e}^{-\beta E_4} \qquad \frac{u}{Z} \to 0 \qquad \frac{v}{Z} \to a_4^2\mathcal{N}_4^2 \tag{18}$$

namely,

$$\mathcal{C}_{12} \to 2\mathcal{N}_4^2 = \frac{2}{2 + a_4^2}. \tag{19}$$

when $\tau \to 0$. In the limit $B \to \infty$, $a_4 \to 0$ and therefore $\mathcal{C}_{12} \to 1$. In the limit $B \to +0$, but $B \gg \tau$, $\mathcal{C}_{12} \to 2/3$.

It is interesting to note that, when $B = 0$, $\mathcal{C}_{12} \to 1/3$ in the limit $\tau \to 0$ [24]. In this case the ground state is three-fold degenerate and the approximation we used above is not valid. This again indicates the role of degeneracy in the entanglement.

4.2. $\mathcal{C}_{13}$

We consider the entanglement between sites 1 and 3. From figures 3 and 4 we see that:

1. In contrast to the 1–2 case, the concurrence increases to a maximum with increasing B and then decreases. The lower the τ, the smaller the B at which the concurrence reaches its maximum value.
2. For small B, entanglement occurs only in the ferromagnetic case ($J < 0$), while for large enough B (e.g. $B = 10$), entanglement occurs in both the antiferromagnetic and ferromagnetic cases, but it is very weak.

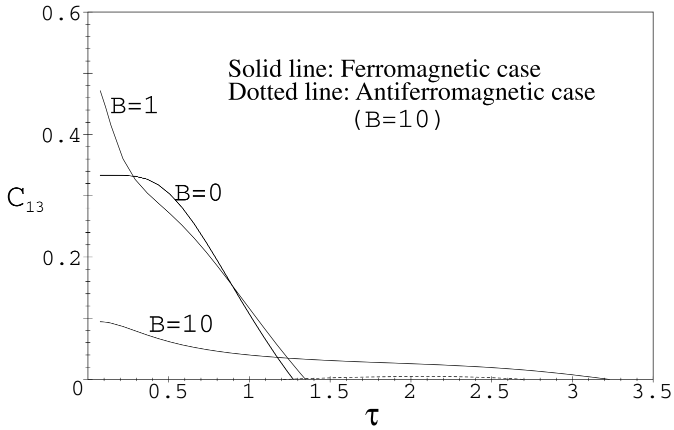

Figure 3. Concurrence $\mathcal{C}_{13}$ against τ for different magnetic fields $B = 0, 1, 10$. For the antiferromagnetic case (dotted line) with $B = 10$, entanglement occurs although it is very weak.

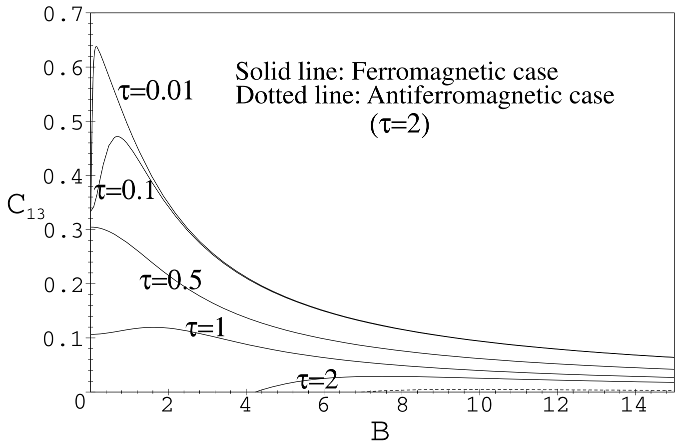

Figure 4. Concurrence $\mathcal{C}_{13}$ against B at different temperatures. For the antiferromagnetic case (dotted line), $\tau = 2$.

Figure 4 suggests that the maximal entanglement occurs in the ferromagnetic case when $\tau \to 0$ and B is also much smaller than 1. In this case, E_1 is very close to the ground state E_4 and $\exp(-\beta E_4)$ and $\exp(-\beta E_1)$ are much larger than others. We can also check that

$$\frac{\mathrm{e}^{-\beta E_4}}{\mathrm{e}^{-\beta E_1}} \sim \exp\left(\frac{2}{3}\frac{B}{\tau}\right) \geqslant 1 \tag{20}$$

and that

$$\mathcal{N}_1 \sim \mathcal{N}_4 \sim \tfrac{1}{3} \qquad a_1 \sim a_4 \sim 1. \tag{21}$$

The concurrence is then given approximately by

$$C_{13} \sim \frac{2}{3}\left[1 - \frac{\exp\left(\frac{1}{3}\frac{B}{\tau}\right)}{1 + \exp\left(\frac{2}{3}\frac{B}{\tau}\right)}\right] \tag{22}$$

from which we conclude that the maximal concurrence is $2/3$ when B is much larger than τ and much smaller than 1.

In summary, we list our results in the following table.

	Maximal concurrence	Entanglement ranges
$B=0$	$1/3$	Antiferromagnetic case only
12	1, when $\|\tau\| \to 0$ and B is large enough	In both ferromagnetic and antiferromagnetic cases
13	$2/3$ for the antiferromagnetic case and $\tau \ll B \ll 1$	When B is small, only the ferromagnetic case is entangled. When B is large enough, both the antiferromagnetic and ferromagnetic cases are entangled, but the entanglement is very weak

5. Conclusion

In this paper we considered the effect of a non-uniform magnetic field on the Heisenberg *XX* model, modelling a magnetic impurity on only one site. In contrast to the uniform magnetic field case [24] where the pairwise thermal entanglement of any two sites is identical due to the *exchange* symmetry of sites, the entanglement due to a non-uniform magnetic field clearly depends on which site the impurity is located. When the impurity is located at the site which is traced out, that is, when it acts as an *external field* of the pair, the concurrence corresponding to the entanglement can be enhanced to the maximal value 1 from $1/3$; while when the field acts on a site of the pair the concurrence can only be increased from $1/3$ to $2/3$. Maximal entanglement is achieved when the temperature tends to zero.

In [24], the entanglement was related to the degeneracy of the system. In the present model, the magnetic field removes all the degeneracy of the energy levels present when $B = 0$ and the entanglement is thus greatly enhanced.

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