Pairwise entanglement in the XX model with a magnetic impurity

Hongchen Fu\textsuperscript{1}∗ Allan I Solomon\textsuperscript{1†} Xiaoguang Wang\textsuperscript{2‡}

\textsuperscript{1}Quantum Processes Group, The Open University, Milton Keynes, MK7 6AA, United Kingdom
\textsuperscript{2}Quantum Information Group, Institute for Scientific Interchange (ISI) Foundation, Viale Settimio Severo 65, I-10133 Torino, Italy

October 26, 2018

Abstract

For a 3-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, modeling 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.

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 entanglement in quantum operations [2, 3, 4] and in indistinguishable fermionic and bosonic systems [3, 5, 6] 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 [3, 7, 8], which have been shown to possess advantages over two-qubit states in quantum teleportation [9], dense coding [10] and quantum cloning [11].

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

∗h.fu@open.ac.uk
†a.i.solomon@open.ac.uk
‡xgwang@isiosf.isi.it
spins [13], electronic spins [20] and optical lattices [21]. By suitable coding, the Heisenberg 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 3-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 3-qubit XX Heisenberg model in a magnetic field acting on the third site only. The Hamiltonian is [25]

$$H = \frac{J}{2} \sum_{i=1}^{3} (\sigma^x_i \sigma^x_{i+1} + \sigma^y_i \sigma^y_{i+1}) + BJ\sigma^z_3,$$

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

$$E_0 = -JB, \quad E_1 = \frac{J}{2} (1 + B_-),$$

$$E_2 = -J(1+B), \quad E_3 = -J(1-B),$$

$$E_4 = \frac{J}{2} (1 + B_+), \quad E_5 = \frac{J}{2} (1 - B_-),$$

$$E_6 = \frac{J}{2} (1 - B_+), \quad E_7 = JB,$$

(2)

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

$$E_1 = E_7 = 0, \quad E_1 = E_3 = E_4 = 2J, \quad E_2 = E_5 = E_6 = -J.$$

(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

$$|\phi_0\rangle = |000\rangle,$$

$$|\phi_1\rangle = \mathcal{N}_1 (|100\rangle + |010\rangle + a_1|001\rangle),$$

$$|\phi_2\rangle = 2^{-1/2} (|010\rangle - |100\rangle),$$

$$|\phi_3\rangle = 2^{-1/2} (|101\rangle - |011\rangle),$$

$$|\phi_4\rangle = \mathcal{N}_4 (a_4|110\rangle + |101\rangle + |011\rangle),$$

$$|\phi_5\rangle = \mathcal{N}_5 (|100\rangle + |010\rangle + a_5|001\rangle),$$

$$|\phi_6\rangle = \mathcal{N}_6 (a_6|110\rangle + |101\rangle + |011\rangle),$$

$$|\phi_7\rangle = |111\rangle,$$

(4)
where
\[
\begin{align*}
a_1 &= -\frac{1}{2} + \frac{1}{2}B_+ + B, \\
a_4 &= -\frac{1}{2} + \frac{1}{2}B_- - B, \\
a_5 &= -\frac{1}{2} - \frac{1}{2}B_+ + B, \\
a_6 &= -\frac{1}{2} - \frac{1}{2}B_- - B,
\end{align*}
\]
(5)
and \(\mathcal{N}_i = (2 + a_i^2)^{-1/2}\) (\(i = 1, 4, 5, 6\)) are normalization constants.

It is interesting to note that the eigenvalues transform under \(B \leftrightarrow -B\) by
\[
\begin{align*}
E_0 &\leftrightarrow E_7, \\
E_1 &\leftrightarrow E_4, \\
E_2 &\leftrightarrow E_3, \\
E_5 &\leftrightarrow E_6,
\end{align*}
\]
(6)
and so the \(a_i\)'s 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
\[
\rho(T) = \frac{1}{Z} \sum_{i=0}^{7} e^{-\beta E_i} |\phi_i\rangle \langle \phi_i|,
\]
(7)
where \(\beta = 1/kT\) and \(Z\) is the partition function
\[
\begin{align*}
Z &= \text{tr} \left( e^{-\beta H} \right) = \sum_{i=0}^{7} e^{-\beta E_i} \\
&= 2(1 + e^{J\beta}) \cosh(J\beta B) + 2e^{-J\beta/2} \left[ \cosh \left( \frac{1}{2} J\beta B_+ \right) + \cosh \left( \frac{1}{2} J\beta B_- \right) \right].
\end{align*}
\]
(9)

3 Concurrence of pairwise entanglement

The easiest way to calculate the entanglement is by means of the concurrence \(C\) between a pair of qubits, which is defined as
\[
C = \max \{ \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0 \},
\]
(10)
where the quantities \(\lambda_i\) are the square roots of the eigenvalues of the operator
\[
\varrho = \rho(\sigma_1^y \otimes \sigma_2^y)^{\rho} (\sigma_1^y \otimes \sigma_2^y)
\]
in descending order; \(\rho\) 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 \(C\), varying between a minimum of zero for \(C = 0\), and a maximum of 1 for \(C = 1\).

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 \(\rho_{13}(\rho_{12})\) of the sites 1 and 3 (1 and 2). Both \(\rho_{12}\) and \(\rho_{13}\) take the following form
\[
\rho = \frac{1}{Z} \begin{pmatrix}
u & u & w_1 & y \\
w_1 & y & w_2 & v \\
y & w_2 & u & w_1 \\
v & w_1 & w_2 & u
\end{pmatrix}
\]
(12)
Here, for $\rho_{12}$, the nonzero matrix elements are given by

$$
\begin{align*}
    y &= N_2^2 e^{-\beta E_1} + N_4^2 e^{-\beta E_4} + N_5^2 e^{-\beta E_5} + N_6^2 e^{-\beta E_6} \\
    &\quad - \frac{1}{2} e^{-\beta E_2} - \frac{1}{2} e^{-\beta E_3} \\
    w_1 = w_2 &= N_1^2 e^{-\beta E_1} + N_4^2 e^{-\beta E_4} + N_5^2 e^{-\beta E_5} + N_6^2 e^{-\beta E_6} \\
    &\quad + \frac{1}{2} e^{-\beta E_2} + \frac{1}{2} e^{-\beta E_3} \\
    u &= e^{-\beta E_0} + a_1^2 N_1^2 e^{-\beta E_1} + a_5^2 N_5^2 e^{-\beta E_5}, \\
    v &= e^{-\beta E_7} + a_4^2 N_4^2 e^{-\beta E_4} + a_6^2 N_6^2 e^{-\beta E_6}.
\end{align*}
$$

while for the $\rho_{13}$ case, we have

$$
\begin{align*}
    y &= a_1 N_1^2 e^{-\beta E_1} + a_4 N_4^2 e^{-\beta E_4} + a_5 N_5^2 e^{-\beta E_5} + a_6 N_6^2 e^{-\beta E_6} \\
    w_1 &= a_2 N_2^2 e^{-\beta E_2} + N_2^2 e^{-\beta E_4} + a_5^2 N_5^2 e^{-\beta E_5} + N_6^2 e^{-\beta E_6} \\
    w_2 &= N_1^2 e^{-\beta E_1} + \frac{1}{2} e^{-\beta E_2} + a_2 N_2^2 e^{-\beta E_4} + N_5^2 e^{-\beta E_5} + a_6^2 N_6^2 e^{-\beta E_6} \\
    u &= e^{-\beta E_0} + N_1^2 e^{-\beta E_1} + \frac{1}{2} e^{-\beta E_2} + N_5^2 e^{-\beta E_5}, \\
    v &= e^{-\beta E_7} + \frac{1}{2} e^{-\beta E_3} + N_1^2 e^{-\beta E_1} + N_6^2 e^{-\beta E_6}.
\end{align*}
$$

The concurrence has the form

$$
C = \frac{2}{Z} \max \left\{ |y| - \sqrt{uv}, 0 \right\}.
$$

The system is entangled when $C > 0$, and maximally entangled when $C = 1$. 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 $\tau \equiv kT/|J| \geq 0$. The concurrence is a function of $\tau$ and $B$.

From Eqs. (13) it is easy to see that $y \rightarrow y$ and $u \leftrightarrow v$ when $B \rightarrow -B$. This means that the concurrence is invariant under $B \leftrightarrow -B$;

$$
C(\tau, B) = C(\tau, -B).
$$

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

## 4 Discussion and results

### 4.1 $C_{12}$

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

4
Fig. 1 also suggests that the concurrence $C_{12}$ 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 $e^{-\beta E_2} \gg e^{-\beta E_i}$ for $i \neq 2$ in the limit $\tau \to 0$. Note that all $N_i$ and $a_i$ are finite. Then we have

\begin{align}
y \to \frac{1}{2} e^{-\beta E_2}, \quad Z \to e^{-\beta E_2}, \quad \frac{u}{Z} \to 0, \quad \frac{v}{Z} \to 0,
\end{align}

namely, $C_{12} \to 1$ 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 $e^{-\beta E_4} \gg e^{-\beta E_i}$ ($i \neq 4$) in the limit $\tau \to 0$. Then we have

\begin{align}
y \to N_4^2 e^{-\beta E_4}, \quad Z \to e^{-\beta E_4}, \quad \frac{u}{Z} \to 0, \quad \frac{v}{Z} \to a_4^2 N_4^2,
\end{align}

namely,

\begin{align}
C_{12} \to 2N_4^2 = \frac{2}{2 + a_4^2}.
\end{align}

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

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

### 4.2 $C_{13}$

We consider the entanglement between sites 1 and 3. From Fig. 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 $\tau$, the smaller $B$ 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.

Fig. 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 bigger than others. We can also check that

\begin{align}
\frac{e^{-\beta E_4}}{e^{-\beta E_1}} \sim \exp\left(\frac{2}{3} \frac{B}{\tau}\right) \geq 1,
\end{align}

and that

\begin{align}
N_1 \sim N_4 \sim \frac{1}{3}, \quad a_1 \sim a_4 \sim 1.
\end{align}

The concurrence is then given approximately by

\begin{align}
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],
\end{align}
from which we conclude that the maximal concurrence is $2/3$ when $B$ is much bigger than $\tau$ and much smaller than 1.

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

| B | Maximal concurrence | Entanglement ranges |
|---|---------------------|---------------------|
| 0 | 1/3                 | Antiferromagnetic case only |
| 12 | $1$, when $|\tau| \to 0$ and $B$ is big enough. | In both ferromagnetic and antiferromagnetic cases |
| 13 | $2/3$ for antiferromagnetic case and $\tau \ll B \ll 1$ | When $B$ is small, only the ferromagnetic case is entangled. When $B$ is big 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, modeling 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 on 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.

6 Acknowledgement

X. Wang is supported by European project Q-ACTA.

References

[1] Bennett C H and DiVincenzo D P 2000 Nature 404 247.

[2] Zanardi P, Zalka C and Faoro L 2000 Phys. Rev. A 62 030301; Zanardi P 2001 Phys. Rev. A 63 040304.

[3] Dür W, Vidal G, Cirac J I, Linden N and Popescu S, quant-ph/0006034.

[4] Cirac J I, Dür W, Kraus B and Lewenstein M 2001 Phys. Rev. Lett. 86 544.

[5] Schliemann J, Cirac J I, Kuš M, Lewenstein M and Loss D 2001 Phys. Rev. A 64 022303 (quant-ph/0012094).
[6] Li Y S, Zeng B, Liu X S and Long G L 2001 Phys. Rev. A 64 054302 (quant-ph/0104101).
[7] Zanardi P 2002 Phys. Rev. A 65 in press (quant-ph/0104114).
[8] Dür W, Vidal G and Cirac J I 2000 Phys. Rev. A 62 062314.
[9] Coffman V, Kundu J and Wootters W K 2000 Phys. Rev. A 61 052306; Sudbery A 2001 J. Phys. A 34 643; Carteret H A and Sudbery A, quant-ph/0001091; Brun T A and Cohen O 2001 Phys. Lett. A 281; Acín A, Andrianov A, Costa L, Jané E, Latorre J I and Tarrach R 2000 Phys. Rev. Lett. 85 1560; Acín A, Andrianov A, Jané E and Tarrach R, quant-ph/0009107.
[10] Rajagopal A K and Rendell R W, quant-ph/0104122.
[11] Karlsson A and Bourennane M 1998 Phys. Rev. A 58 4394; Gorbachev V N and Trubilko A I 2000 JETP 91 894.
[12] Hao J C, Li C F and Guo G C 2001 Phys. Rev. A 63 054301.
[13] BrußD, DiVincenzo D P, Ekert A, Fuchs C A, Macchiavello C and Smolin J A 1998 Phys. Rev. A 57 2368.
[14] Nielsen M A 1998 Ph. D thesis, University of Mexico, quant-ph/0011036; Arnesen M C, Bose S and Vedral V 2001 Phys. Rev. Lett. 87 017901 (quant-ph/0009060).
[15] Wang X 2001 Phys. Rev. A 64 012313.
[16] Wang X 2001 Phys. Lett. A 281 101.
[17] Gunlycke D, Bose S, Kendon V M and Vedral V, 2001 Phys. Rev. A 64 042302 (quant-ph/0102137).
[18] Loss D and Divincenzo D P 1998 Phys. Rev. A 57 120; Burkard G, Loss D and DiVincenzo D P 1999 Phys. Rev. B 59 2070.
[19] Kane B E 1998 Nature 393 133.
[20] Vrijen R, Yablonovitch E, Wang K, Jiang H, Balandin A, Roychowdhury V, Mor T, DiVincenzo D, quant-ph/9905096.
[21] Sørensen A and Mølmer A 1999 Phys. Rev. Lett. 83 2274.
[22] Lidar D A, Bacon D and Whaley K B 1999 Phys. Rev. Lett. 82 4556; DiVincenzo D P, Bacon D, Kempe J, Burkard G and Whaley K B 2000 Nature 408 339.
[23] O’Connor K M, Wootters W K 2001 Phys. Rev. A 63 052302.
[24] Wang X, Fu H and Solomon A I 2001 J. Phys. A 34 11307.
[25] Lieb E, Schultz T and Mattis D 1961 Ann. Phys. (N. Y.) 16 407.
[26] Hill S and Wootters W K 1997 Phys. Rev. Lett. 78 5022; Wootters W K 1998 Phys. Rev. Lett. 80 2245; Coffman V, Kundu J and Wootters W K 2000 Phys. Rev. A 61 052306.
Figure 1: Concurrence $C_{12}$ against $\tau$ for different magnetic field $B = 0, 1, 10$.

Figure 2: Concurrence $C_{12}$ against $B$ at different temperature $\tau = 0.1, 0.5$ and 1.
Figure 3: Concurrence $C_{13}$ against $\tau$ for different magnetic field $B = 0, 1, 10$. For antiferromagnetic case (dotted line) with $B = 10$, the entanglement occurs although it is very week.

Figure 4: Concurrence $C_{13}$ against $B$ at different temperature. For antiferromagnetic case (dotted line), $\tau = 2$. 