Eur. Phys. J. D **41**, 571–578 (2007)
DOI: 10.1140/epjd/e2006-00271-3

THE EUROPEAN PHYSICAL JOURNAL D

Entanglement in the three-qubit Heisenberg model with next nearest neighbor interaction and a nonuniform magnetic field

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Received 25 August 2006 / Received in final form 17 October 2006
Published online 15 December 2006 –

Abstract. Pairwise thermal entanglement in the three-qubit *XXX* Heisenberg model with next nearest neighbor interaction and a nonuniform magnetic field has been studied. It's found that the next nearest neighbor interaction has a great effect on the entanglement between the next nearest neighbor sites, but has slight effect on the nearest neighbor entanglement (NNE). Applying a magnetic field at the middle site enhances the next nearest neighbor entanglement (NNNE) sharply when there is a small field at the side sites and the next nearest neighbor coupling constant is positive. A staggered magnetic field helps to maintain nearest neighbor entanglement obviously.

PACS. 42.50.Dv Nonclassical states of the electromagnetic field, including entangled photon states; quantum state engineering and measurements – 03.67.-a Quantum information – 03.65.Ud Entanglement and quantum nonlocality (e.g. EPR paradox, Bell's inequalities, GHZ states, etc.)

QICS. 03.40.+t Thermal/mixed state entanglement – 04.10.+s Entanglement in spin models

1 Introduction

One of the amusing properties of quantum mechanics is the entanglement. Entangled states of component systems and their unique properties have attracted a lot of attention since the early days [1–4]. Entanglement is responsible for the non-local correlations, which can exist between spatially separated quantum systems. Recently, it's found that entanglement plays a very important role in quantum information processing, such as quantum teleportation [5], superdense coding [6], quantum computation [7,8] and some cryptographic protocols [9,10]. For a pair of qubits, the entanglement is rigorously described by the concurrence [11,12]

$$C = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\} \tag{1.1}$$

where λ_i $(i = 1, 2, 3, 4)$ are the positive square roots of the operator

$$R = \rho\,(\sigma_1^y \otimes \sigma_2^y)\,\rho^*\,(\sigma_1^y \otimes \sigma_2^y) \tag{1.2}$$

in the descending order and ρ is the density matrix. The concurrence (1.1) can be rewritten as

$$C = \max\left\{0, \left[2\max(\lambda_1, \lambda_2, \lambda_3, \lambda_4) - \sum_{i=1}^{4}\lambda_i\right]\right\}. \tag{1.3}$$

This form of the concurrence will be used in the following calculations. Extensive studies on the thermal entanglement (entanglement at finite temperature) in Heisenberg spin models [13–30] have been done. The Heisenberg spin chain has been used to construct a quantum computer and quantum dots [31], nuclear spins [32], electronic spins [33] and optical lattices [34]. By proper coding, the Heisenberg interaction alone can be used for quantum computation [35–37].

In this article, we focus our attention on the three-qubit *XXX* chain with next nearest neighbor interaction and a nonuniform magnetic field. Effects on NNE and NNNE by the next nearest neighbor coupling constant and the magnetic field are studied. To our knowledge, no one has done such a discussion before. The discussions are arranged as follows. The next section is the model and the exact solution. The third section deals with the case of finite temperature. The final section is the conclusion.

2 The model and the exact solution

For the three-qubit *XXX* chain under external magnetic fields and with next nearest neighbor interaction, the Hamiltonian is

$$\begin{aligned} H = J\vec{S}_1 \cdot \vec{S}_2 + J\vec{S}_2 \cdot \vec{S}_3 + J'\vec{S}_1 \cdot \vec{S}_3 \\ - S_{1z}B - S_{3z}B - S_{2z}b \end{aligned} \tag{2.1}$$

where b is the magnetic field at the middle site, B the magnetic field at the other two sites, J and J' are the coupling constants between nearest neighbors and the next nearest neighbor sites respectively. The Schrödinger equation $H|\psi\rangle = E|\psi\rangle$ can be solved this way. Defining two

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$$A_1 = \frac{J}{\sqrt{\frac{9}{4}J^2 + (b-B)^2 - J(b-B) + \left(b - B - \frac{1}{2}J\right)\sqrt{(b-B)^2 - (b-B)J + \frac{9}{4}J^2}}}$$

$$A_2 = \frac{J}{\sqrt{\frac{9}{4}J^2 + (b-B)^2 - J(b-B) - \left(b - B - \frac{1}{2}J\right)\sqrt{(b-B)^2 - (b-B)J + \frac{9}{4}J^2}}}$$

$$D_1 = \frac{\frac{1}{2}(b-B) - \frac{1}{4}J + \frac{1}{2}\sqrt{(b-B)^2 - (b-B)J + \frac{9}{4}J^2}}{\sqrt{\frac{9}{8}J^2 + \frac{1}{2}(b-B)^2 - \frac{1}{2}J(b-B) + \frac{1}{2}\left(b - B - \frac{1}{2}J\right)\sqrt{(b-B)^2 - (b-B)J + \frac{9}{4}J^2}}}$$

$$D_2 = \frac{\frac{1}{2}(b-B) - \frac{1}{4}J - \frac{1}{2}\sqrt{(b-B)^2 - (b-B)J + \frac{9}{4}J^2}}{\sqrt{\frac{9}{8}J^2 + \frac{1}{2}(b-B)^2 - \frac{1}{2}J(b-B) - \frac{1}{2}\left(b - B - \frac{1}{2}J\right)\sqrt{(b-B)^2 - (b-B)J + \frac{9}{4}J^2}}}$$

$$B_1 = \frac{J}{\sqrt{\frac{9}{4}J^2 + (B-b)^2 - J(B-b) + \left(B - b - \frac{1}{2}J\right)\sqrt{(B-b)^2 - (B-b)J + \frac{9}{4}J^2}}}$$

$$B_2 = \frac{J}{\sqrt{\frac{9}{4}J^2 + (B-b)^2 - J(B-b) - \left(B - b - \frac{1}{2}J\right)\sqrt{(B-b)^2 - (B-b)J + \frac{9}{4}J^2}}}$$

$$F_1 = \frac{\frac{1}{2}(B-b) - \frac{1}{4}J + \frac{1}{2}\sqrt{(B-b)^2 - (B-b)J + \frac{9}{4}J^2}}{\sqrt{\frac{9}{8}J^2 + \frac{1}{2}(B-b)^2 - \frac{1}{2}J(B-b) + \frac{1}{2}\left(B - b - \frac{1}{2}J\right)\sqrt{(B-b)^2 - (B-b)J + \frac{9}{4}J^2}}}$$

$$F_2 = \frac{\frac{1}{2}(B-b) - \frac{1}{4}J - \frac{1}{2}\sqrt{(B-b)^2 - (B-b)J + \frac{9}{4}J^2}}{\sqrt{\frac{9}{8}J^2 + \frac{1}{2}(B-b)^2 - \frac{1}{2}J(B-b) - \frac{1}{2}\left(B - b - \frac{1}{2}J\right)\sqrt{(B-b)^2 - (B-b)J + \frac{9}{4}J^2}}} \quad (2.3)$$

operators $\vec{L} = \vec{S}_1 + \vec{S}_3$ and $\vec{J} = \vec{L} + \vec{S}_2$, one can prove that $\vec{L}^2$, J_z and H commute with one another. Writing the eigenvalue of $\vec{L}^2$ as $l(l+1)$, the possible values for l are 0 and 1. The possible eigenvalues for J_z are $m = \pm 1/2,\ \pm 3/2$ as the total spin for three spin-1/2 particles is 1/2 and 3/2. Using $|l, m, E\rangle$ to represent the eigenstates of the system, we find that $|1, 1/2, E\rangle$ is the superposition of $|1_1 1_3 0_2\rangle$ and $(|1_1 0_3\rangle + |0_1 1_3\rangle)|1_2\rangle\sqrt{2}$. The superstition coefficients and the energy are not difficult to get from the Schrödinger equation. The eigenstates are identified as $|\psi_1\rangle = |1, 1/2, E_1\rangle$ and $|\psi_2\rangle = |1, 1/2, E_2\rangle$. In a similar way, we can find $|1, -1/2, E\rangle$, which is the superposition of $|0_1 0_3 1_2\rangle$ and $(|1_1 0_3\rangle + |0_1 1_3\rangle)|0_2\rangle\sqrt{2}$. The corresponding eigenstates are identified as $|\psi_3\rangle = |1, -1/2, E_3\rangle$ and $|\psi_4\rangle = |1, -1/2, E_4\rangle$. The other eigenstates are easier to get $|1, 3/2, E_5\rangle = |1_1 1_3 1_2\rangle = |\psi_5\rangle$, $|1, -3/2, E_6\rangle = |0_1 0_3 0_2\rangle = |\psi_6\rangle$, $|0, 1/2, E_7\rangle = (|1_1 0_3\rangle - |0_1 1_3\rangle)|1_2\rangle/\sqrt{2} = |\psi_7\rangle$ and $|0, -1/2, E_8\rangle = (|1_1 0_3\rangle - |0_1 1_3\rangle)|0_2\rangle/\sqrt{2} = |\psi_8\rangle$. The eigenfunctions are finally found to be ($|\psi_j\rangle$, $j = 5 \to 8$ are not listed)

$$|\psi_1\rangle = A_1(|1_1 0_3\rangle + |0_1 1_3\rangle)|1_2\rangle/\sqrt{2} + D_1|1_1 1_3 0_2\rangle$$

$$|\psi_2\rangle = A_2(|1_1 0_3\rangle + |0_1 1_3\rangle)|1_2\rangle/\sqrt{2} + D_2|1_1 1_3 0_2\rangle$$

$$|\psi_3\rangle = B_1(|1_1 0_3\rangle + |0_1 1_3\rangle)|0_2\rangle/\sqrt{2} + F_1|0_1 0_3 1_2\rangle$$

$$|\psi_4\rangle = B_2(|1_1 0_3\rangle + |0_1 1_3\rangle)|0_2\rangle/\sqrt{2} + F_2|0_1 0_3 1_2\rangle \quad (2.2)$$

where the coefficients are

see equations (2.3) above.

The corresponding energy eigenvalues are respectively

$$E_1 = \frac{1}{4}(J' - J) - \frac{1}{2}B + \frac{1}{2}\sqrt{(b-B)^2 - (b-B)J + \frac{9}{4}J^2}$$

$$E_2 = \frac{1}{4}(J' - J) - \frac{1}{2}B - \frac{1}{2}\sqrt{(b-B)^2 - (b-B)J + \frac{9}{4}J^2}$$

$$E_3 = \frac{1}{4}(J' - J) + \frac{1}{2}B + \frac{1}{2}\sqrt{(B-b)^2 - (B-b)J + \frac{9}{4}J^2}$$

$$E_4 = \frac{1}{4}(J' - J) + \frac{1}{2}B - \frac{1}{2}\sqrt{(B-b)^2 - (B-b)J + \frac{9}{4}J^2}$$

$$E_5 = \frac{1}{4}J' + \frac{1}{2}J - B - \frac{1}{2}b$$

$$E_6 = \frac{1}{4}J' + \frac{1}{2}J + B + \frac{1}{2}b$$

$$E_7 = -\frac{3}{4}J' - \frac{1}{2}b$$

$$E_8 = -\frac{3}{4}J' + \frac{1}{2}b. \quad (2.4)$$

Clearly, $|\psi_5\rangle$ and $|\psi_6\rangle$ are disentangled states. For $|\psi_7\rangle$ and $|\psi_8\rangle$, qubits 1 and 3 are maximally entangled, but qubit 2 is not entangled with the other two. For the other four eigenstates, the three qubits are entangled with one another. The next nearest neighbor coupling constant J' only appears in the energy eigenvalues. The difference $B - b$ between the magnetic fields B and b influences the eigenstates. In case of $B = b$ or a uniform magnetic field, the eigenstates are not affected.

3 Thermal entanglement

At finite temperature, the density operator of the system is

$$\rho(T) = \exp(-H/kT)/Z \quad (3.1)$$

where $Z = \mathrm{Tr}[\exp(-H/kT)] = \sum_{i=1}^{8}\exp(-E_i/kT)$ is the partition function. First, let's deal with NNE. From (3.1), we get $\rho_{12}(T) = \mathrm{Tr}_3\rho$. Under the basis $|0_1 0_2\rangle$, $|0_1 1_2\rangle$, $|1_1 0_2\rangle$ and $|1_1 1_2\rangle$, we have the matrix form for $\rho_{12}(T)$

$$\rho_{12}(T) = \frac{1}{Z}\begin{bmatrix} p_1 & 0 & 0 & 0 \\ 0 & u & w & 0 \\ 0 & w & v & 0 \\ 0 & 0 & 0 & p_2 \end{bmatrix} \quad (3.2a)$$

where

$$p_1 = \frac{B_1^2}{2}\exp\left(-\frac{E_3}{T}\right) + \frac{B_2^2}{2}\exp\left(-\frac{E_4}{T}\right) + \exp\left(-\frac{E_6}{T}\right) + \frac{1}{2}\exp\left(-\frac{E_8}{T}\right)$$

$$p_2 = \frac{A_1^2}{2}\exp\left(-\frac{E_1}{T}\right) + \frac{A_2^2}{2}\exp\left(-\frac{E_2}{T}\right) + \exp\left(-\frac{E_5}{T}\right) + \frac{1}{2}\exp\left(-\frac{E_7}{T}\right)$$

$$u = \frac{A_1^2}{2}\exp\left(-\frac{E_1}{T}\right) + \frac{A_2^2}{2}\exp\left(-\frac{E_2}{T}\right) + F_1^2\exp\left(-\frac{E_3}{T}\right) + F_2^2\exp\left(-\frac{E_4}{T}\right) + \frac{1}{2}\exp\left(-\frac{E_7}{T}\right)$$

$$v = \frac{B_1^2}{2}\exp\left(-\frac{E_3}{T}\right) + \frac{B_2^2}{2}\exp\left(-\frac{E_4}{T}\right) + D_1^2\exp\left(-\frac{E_1}{T}\right) + D_2^2\exp\left(-\frac{E_2}{T}\right) + \frac{1}{2}\exp\left(-\frac{E_8}{T}\right)$$

$$w = \frac{A_1 D_1}{\sqrt{2}}\exp\left(-\frac{E_1}{T}\right) + \frac{A_2 D_2}{\sqrt{2}}\exp\left(-\frac{E_2}{T}\right) + \frac{B_1 F_1}{\sqrt{2}}\exp\left(-\frac{E_3}{T}\right) + \frac{B_2 F_2}{\sqrt{2}}\exp\left(-\frac{E_4}{T}\right). \quad (3.2b)$$

By some calculations, the square roots of the operator (1.2) are found to be $\sqrt{p_1 p_1}/Z$, $\sqrt{p_1 p_1}/Z$, $|w + \sqrt{uv}|/Z$ and $|w - \sqrt{uv}|/Z$. From (1.3), the concurrence is obtained

$$C_{12}(T) = \max\left\{0, \left[2\max\left(\frac{\sqrt{p_1 p_2}}{Z}, \frac{|w+\sqrt{uv}|}{Z}, \frac{|w-\sqrt{uv}|}{Z}\right) - 2\frac{\sqrt{p_1 p_2}}{Z} - \frac{|w+\sqrt{uv}|}{Z} - \frac{|w-\sqrt{uv}|}{Z}\right]\right\}. \quad (3.3)$$

Calculations also show that $C_{12}(T) = C_{23}(T)$.

Here we consider the effects of the magnetic fields and the next nearest neighbor interaction. The temperature effects will be given at the end of this section. The concurrence $C_{12}(T)$ as a function of the magnetic fields B and b is plotted in Figure 1 for $J = 1$ or the antiferromagnetic case. For smaller magnetic fields, the entanglement is larger. When B and b are in the same direction, the entanglement drops to zero rapidly. However, if B and b are in the opposite direction, the entanglement will keep nonzero for a larger scale. The concurrence is symmetry about the lines $B = b$ (the uniform magnetic field) and $B = -b$ (non-uniform or a staggered field), which is similar to the former results [13–20]. Comparing Figure 1b with 1a, one sees that the next nearest neighbor interaction has slight effect on the concurrence.

Figure 2 gives the nearest neighbor concurrence for $J = -1$ or the ferromagnetic case. When there is no magnetic field, the concurrence is zero, which can also be seen clearly from Figure 3. A little increase in the magnetic fields makes the concurrence increase quickly. The concurrence decreases when the magnetic fields further increase.

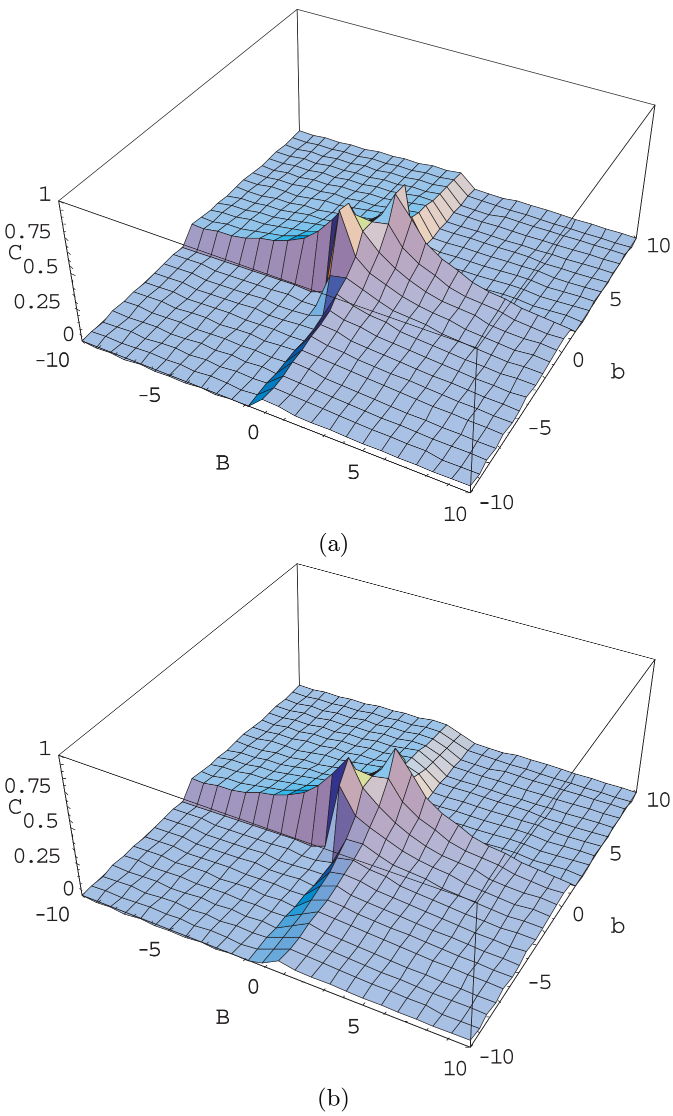


Fig. 1. (Color online) The concurrence C_{12} versus the magnetic fields B and b for $J = 1$, $T = 0.05$ and (a) $J' = 0$, (b) $J' = 0.5$.

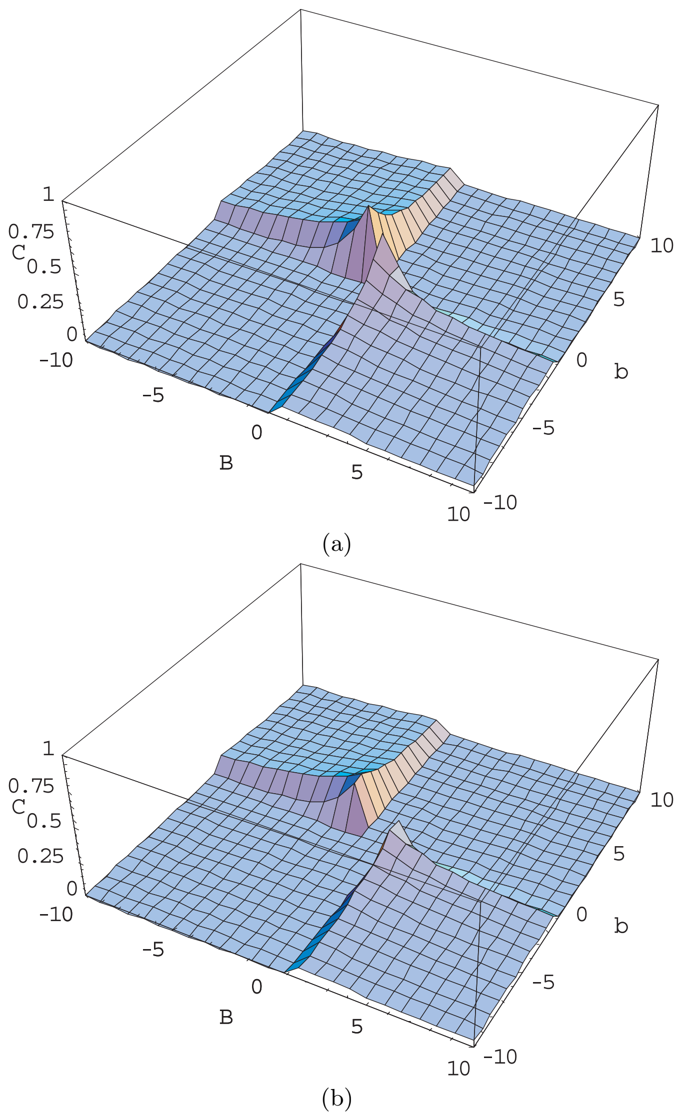


Fig. 2. The concurrence $C_{12}(T)$ versus the magnetic fields B and b for $J = -1$, $T = 0.05$ and (a) $J' = 0$, (b) $J' = 0.8$.

From the figures, we also notice that the next nearest neighbor interaction reduces the concurrence and makes the central area that there is no entanglement become larger.

To see the entanglement at the centre in Figure 2a, the change of the entanglement with the magnetic field when $B = -b$ is plotted in Figure 3. One sees clearly that at the centre, the entanglement is zero.

Now, let's turn to the entanglement between the next nearest neighbor qubits. From (3.1), we obtain $\rho_{13}(T) = \mathrm{Tr}_2\rho$. Under the basis $|0_1 0_3\rangle$, $|0_1 1_3\rangle$, $|1_1 0_3\rangle$ and $|1_1 1_3\rangle$, we have

$$\rho_{13}(T) = \frac{1}{Z}\begin{bmatrix} q_1 & 0 & 0 & 0 \\ 0 & x & y & 0 \\ 0 & y & x & 0 \\ 0 & 0 & 0 & q_2 \end{bmatrix} \tag{3.4a}$$

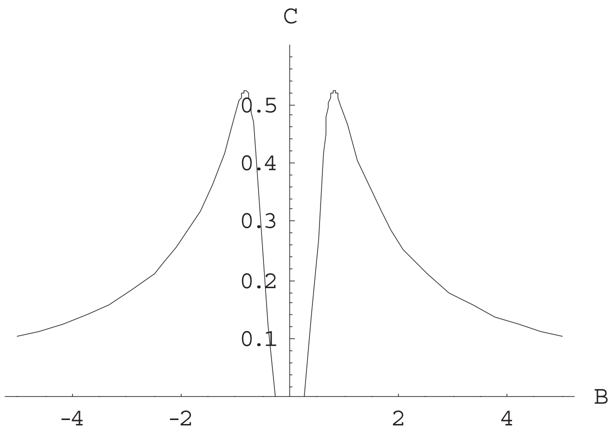


Fig. 3. The concurrence C_{12} is plotted as a function of the magnetic field B when $b = -B$ and $J = -1$, $T = 0.05$, $J' = 0$.

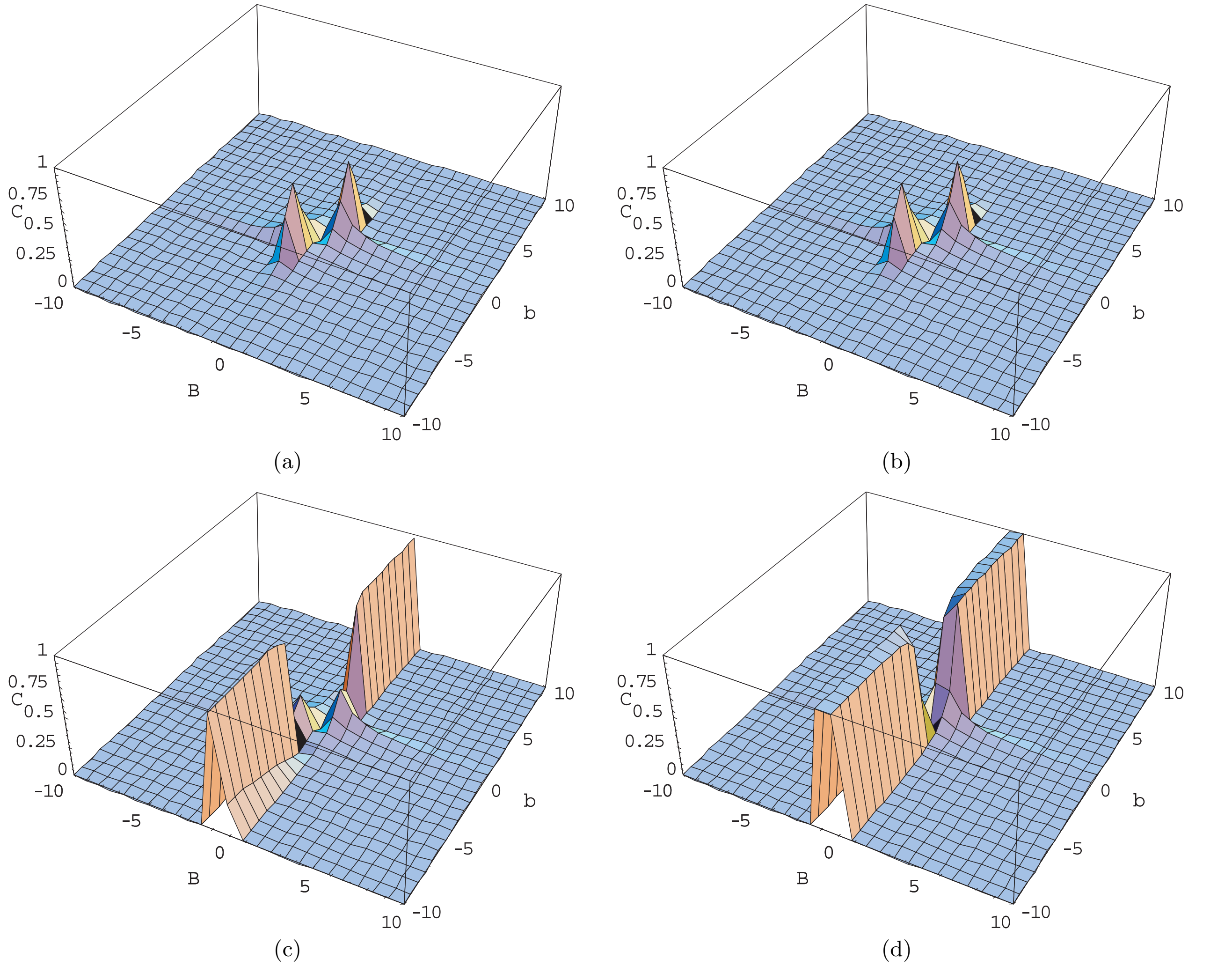


Fig. 4. (Color online) The concurrence C_{13} versus the magnetic fields B and b for $J = 1$, $T = 0.05$ and (a) $J' = -0.5$, (b) $J' = 0$, (c) $J' = 0.5$, (d) $J' = 0.8$.

where the coefficients are

see equations (3.4b) below.

Further, square roots of the operator (1.2) can be found, which are $\sqrt{q_1 q_2}/Z$, $\sqrt{q_1 q_2}/Z$, $(x+y)/Z$ and $(x-y)/Z$.

The concurrence is then

$$C_{13}(T) = \max\left\{0, \left[2\max\left(\frac{\sqrt{q_1 q_2}}{Z}, \frac{(x+y)}{Z}, \frac{(x-y)}{Z}\right) -2\frac{\sqrt{q_1 q_2}}{Z} - \frac{(x+y)}{Z} - \frac{(x-y)}{Z}\right]\right\}. \quad (3.5)$$

$$q_1 = F_1^2 \exp\left(-\frac{E_3}{T}\right) + F_2^2 \exp\left(-\frac{E_4}{T}\right) + \exp\left(-\frac{E_6}{T}\right), \qquad q_2 = D_1^2 \exp\left(-\frac{E_1}{T}\right) + D_2^2 \exp\left(-\frac{E_2}{T}\right) + \exp\left(-\frac{E_5}{T}\right)$$

$$x = \frac{A_1^2 \exp\left(-\frac{E_1}{T}\right) + A_2^2 \exp\left(-\frac{E_2}{T}\right) + B_1^2 \exp\left(-\frac{E_3}{T}\right) + B_2^2 \exp\left(-\frac{E_4}{T}\right) + \exp\left(-\frac{E_7}{T}\right) + \exp\left(-\frac{E_8}{T}\right)}{2}$$

$$y = \frac{A_1^2 \exp\left(-\frac{E_1}{T}\right) + A_2^2 \exp\left(-\frac{E_2}{T}\right) + B_1^2 \exp\left(-\frac{E_3}{T}\right) + B_2^2 \exp\left(-\frac{E_4}{T}\right) - \exp\left(-\frac{E_7}{T}\right) - \exp\left(-\frac{E_8}{T}\right)}{2} \quad (3.4b)$$

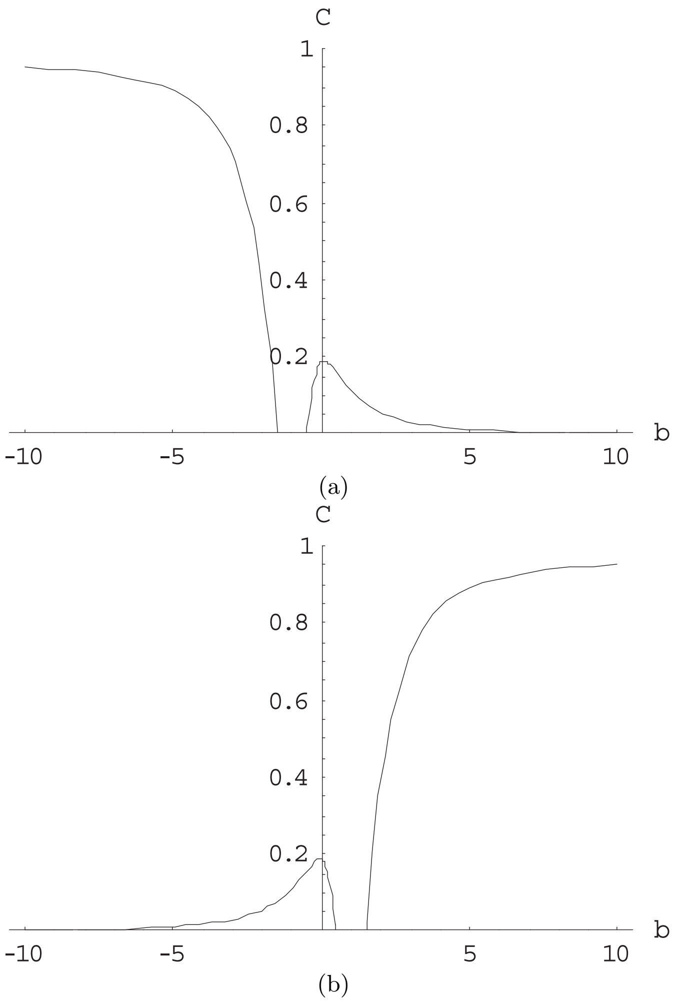


Fig. 5. The concurrence C_{13} is plotted as a function of the magnetic fields B and b when $J = 1$, $T = 0.05$, $J' = 0.5$ and (a) $B = -0.2$, (b) $B = 0.2$.

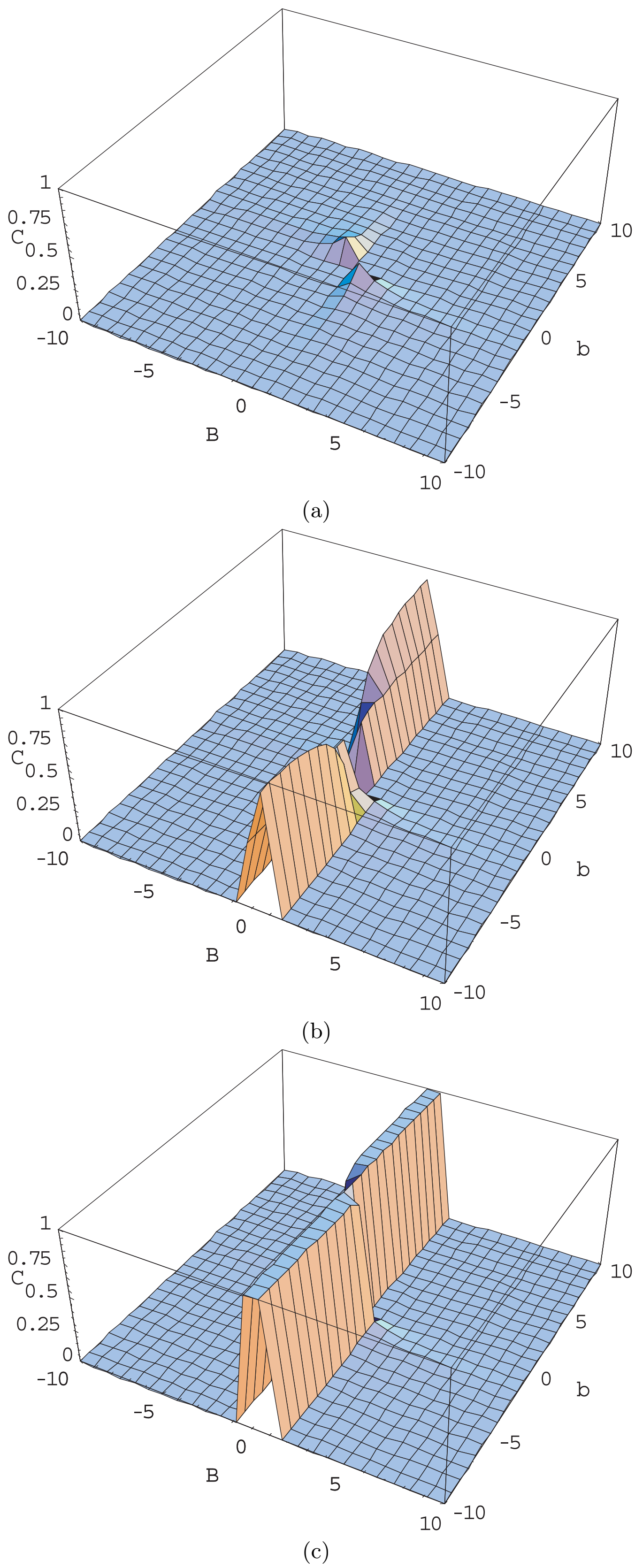


Fig. 6. (Color online) The concurrence C_{13} versus the magnetic fields B and b for $J = -1$, $T = 0.05$ and (a) $J' = 0$, (b) $J' = 0.5$, (c) $J' = 0.8$.

The next nearest neighbor concurrence as a function of the magnetic fields B and b is plotted in Figure 4 for $J = 1$. When J' is negative, it has little effect on the concurrence. However, when J' is positive, it makes the concurrence increase quickly when there is a large magnetic field at the middle site and a small field at the side sites, which can be seen more clearly from Figure 5. Such a phenomenon of the concurrence we haven't seen from former studies [13–30]. For positive J', the concurrence is no longer symmetry about the lines $B = b$ (the uniform magnetic field) and $B = -b$ (non-uniform or a staggered field), which is different from the former results [13–20].

In Figure 5, the concurrence as a function of b is plotted when a fixed value of B is taken. One sees that B behaves like a biased field. When b is in the same direction with B, the concurrence increases greatly.

For $J = -1$, the concurrence has similar behaviors as shown in Figure 6. For negative and zero J', the concurrence is very small. For positive J', the concurrence can be increased greatly by applying a magnetic field at the middle site.

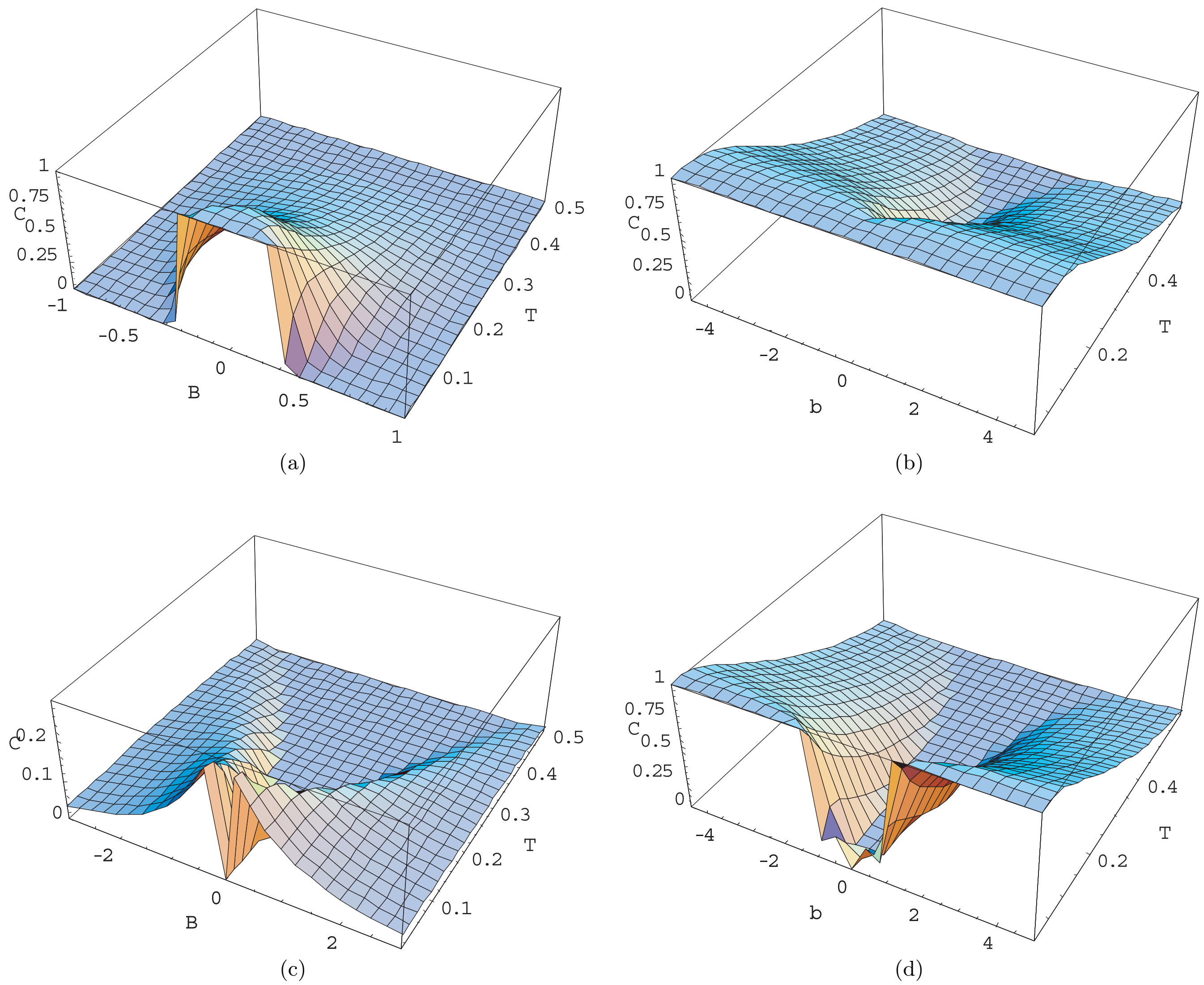


Fig. 7. (Color online) The concurrence C_{13} is plotted as a function of magnetic field and temperature when $J' = 0.8$ and (a) $J = -1$, $b = 0$, (b) $J = -1$, $B = 0$, (c) $J = 1$, $b = 0$, (d) $J = 1$, $B = 0$.

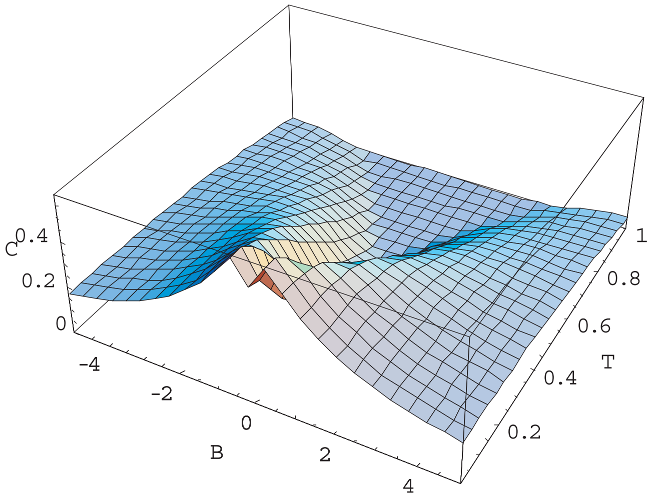
Finally, let's discuss the temperature effects. From the former studies [13–20], we know that increase in the temperature tends to reduce the entanglement, though sometimes the temperature may make the entanglement increase a little (see Fig. 6 in [19]). The concurrence C_{13} as functions of the magnetic field and the temperature is shown in following figures.

In Figure 7c, the concurrence increases a little with the temperature, but finally vanishes with the up-going temperature. One sees from Figures 7b and 7d that a magnetic field at the middle site can slow down the decrease of the entanglement. The nearest neighbor entanglement is shown in Figure 8.

In Figure 8a, there is also the phenomenon that the concurrence increases a little and then drops to zero when the temperature goes up. From Figures 7 and 8 or the former investigations, one sees that a too high temperature always destroys the entanglement. Studying the temperature effects make us know what temperature we should choose to have a proper entanglement.

4 Conclusions

For the three-qubit XXX chain, the next nearest neighbor interaction and different forms of magnetic fields together have important effects on the entanglement. Properly controlling these factors, one can get the entanglement wanted. It is interesting to see the common effects of the next nearest neighbor interaction and magnetic fields in more complex systems such as the four-qubit and five-qubit systems.



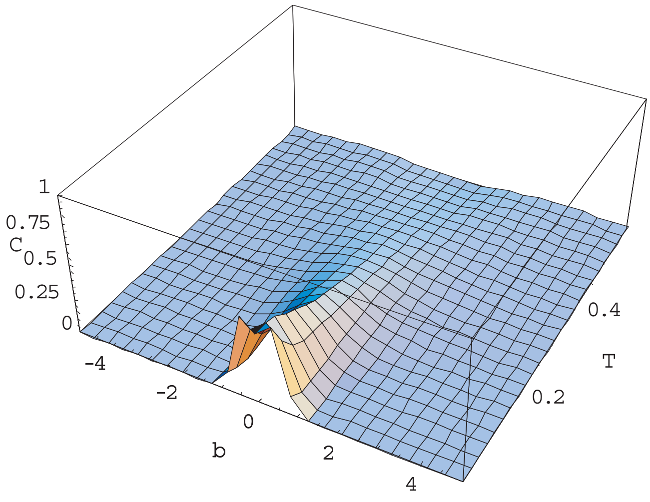


Fig. 8. (Color online) The concurrence C_{12} is plotted as a function of magnetic field and temperature when $J = 1$, $J' = 0.8$ and (a) $b = 0$, (b) $B = 0$.

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