

## Entanglement in spin-1 Heisenberg chains

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2005 J. Phys. A: Math. Gen. 38 8703

(<http://iopscience.iop.org/0305-4470/38/40/014>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.94

The article was downloaded on 03/06/2010 at 03:59

Please note that [terms and conditions apply](#).

# Entanglement in spin-1 Heisenberg chains

Xiaoguang Wang<sup>1</sup>, Hai-Bin Li<sup>2</sup>, Zhe Sun<sup>1</sup> and You-Quan Li<sup>1</sup>

<sup>1</sup> Zhejiang Institute of Modern Physics, Department of Physics, Zhejiang University, HangZhou 310027, People's Republic of China

<sup>2</sup> Department of Applied Physics, Zhejiang University of technology, HangZhou 310014, People's Republic of China

Received 24 March 2005, in final form 3 August 2005

Published 21 September 2005

Online at [stacks.iop.org/JPhysA/38/8703](http://stacks.iop.org/JPhysA/38/8703)

## Abstract

By using the concept of negativity, we study entanglement in spin-1 Heisenberg chains. Both the bilinear chain and the bilinear–biquadratic chain are considered. Due to the  $SU(2)$  symmetry, the negativity can be determined by two correlators, which greatly facilitate the study of entanglement properties. Analytical results of negativity are obtained in the bilinear model up to four spins and in the 2-spin bilinear–biquadratic model, and numerical results of negativity are presented. We determine the threshold temperature before which the thermal state is doomed to be entangled.

PACS numbers: 03.65.Ud, 03.67.–a, 75.10.Jm

## 1. Introduction

Since Haldane's prediction that the one-dimensional Heisenberg chain has a spin gap for integer spins [1], the physics of quantum spin chains has been the subject of many theoretical and experimental studies. In these studies, the bilinear spin-1 Heisenberg model and the bilinear–biquadratic Heisenberg model have played important roles [2–4]. The corresponding Hamiltonians are given by

$$H_1 = \sum_{i=1}^N J \mathbf{S}_i \cdot \mathbf{S}_{i+1}, \quad (1)$$

$$H_2 = \sum_{i=1}^N [J \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \gamma (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2], \quad (2)$$

respectively, where the periodic boundary condition is assumed, namely,  $\mathbf{S}_{N+1} \equiv \mathbf{S}_1$ . Obviously, these two Hamiltonians exhibit a  $SU(2)$  symmetry. Moreover, the bilinear–biquadratic model exhibits a very rich phase diagram [5].

Recently, the study of entanglement properties in Heisenberg systems have received much attention [6–39]. Quantum entanglement lies at the heart of quantum mechanics, and can be exploited to accomplish some physical tasks such as quantum teleportation [40]. Spin-1/2 systems have been considered in most of these studies. However, due to the lack of entanglement measure for higher spin systems, the entanglement in higher spin systems has been less studied. There are several preceding works on entanglement in spin-1 chains. Fan *et al* [33] and Verstraete *et al* [34] studied entanglement in the bilinear–biquadratic model with a special value of  $\gamma = 1/3$ , i.e., the AKLT model [2]. Zhou *et al* studied entanglement in the Hamiltonian  $H_2$  for the case of two spins [35].

In this paper, by using the concept of negativity [41], we study pairwise entanglement in both the bilinear and the bilinear–biquadratic Heisenberg spin-1 models. The negative partial transpose gives a sufficient condition for entanglement of spin-1 particles. The negativity of a 2-spin state  $\rho$  is defined as [41]

$$\mathcal{N}(\rho) = \sum_i |\mu_i|, \quad (3)$$

where  $\mu_i$  is the negative eigenvalue of  $\rho^{T_2}$ , and  $T_2$  denotes the partial transpose with respect to the second system. If  $\mathcal{N} > 0$ , the 2-spin state is entangled.

We study entanglement in both the ground state and the thermal state. The state of a system at thermal equilibrium is described by the density operator  $\rho(T) = \exp(-\beta H)/Z$ , where  $\beta = 1/k_B T$ ,  $k_B$  is Boltzmann's constant, which is assumed to be 1 throughout the paper, and  $Z = \text{Tr}\{\exp(-\beta H)\}$  is the partition function. The entanglement in the thermal state is called thermal entanglement.

We organize the paper as follows. In section 2, we give the exact forms of the negativity for an  $SU(2)$ -invariant state, and show how the negativity is related to the two correlators. We also discuss how to obtain negativity from the ground-state energy and partition function in the bilinear–biquadratic model. We study entanglement in the bilinear and bilinear–biquadratic models in sections 3 and 4, respectively. Some analytical and numerical results of negativity are obtained. We conclude in section 5.

## 2. Negativity and correlators

Schliemann considered the entanglement of two spin-1 particles via the Peres–Horodecki criteria [31], and find that the  $SU(2)$ -invariant state is entangled if either of the following inequalities holds:

$$\langle (\mathbf{S}_i \cdot \mathbf{S}_j)^2 \rangle > 2, \quad \langle (\mathbf{S}_i \cdot \mathbf{S}_j)^2 \rangle + \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle < 1. \quad (4)$$

Now we explicitly give the expression of negativity for the  $SU(2)$ -invariant 2-spin state.

According to the  $SU(2)$ -invariant symmetry, any state of two spin-1 particles has the general form [31]

$$\begin{aligned} \rho = & G |S = 0, S_z = 0\rangle \langle S = 0, S_z = 0| + \frac{H}{3} \sum_{S_z=-1}^1 |S = 1, S_z\rangle \langle S = 1, S_z| \\ & + \frac{1 - G - H}{5} \sum_{S_z=-2}^2 |S = 2, S_z\rangle \langle S = 2, S_z|, \end{aligned} \quad (5)$$

where  $|S, S_z\rangle$  denotes a state of total spin  $S$  and  $z$  the component of  $S_z$ , and

$$G = \frac{1}{3}[\langle (\mathbf{S}_i \cdot \mathbf{S}_j)^2 \rangle - 1], \quad H = 1 - \frac{1}{2}[\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle + \langle (\mathbf{S}_i \cdot \mathbf{S}_j)^2 \rangle]. \quad (6)$$

In order to perform partial transpose, the product basis spanned by  $\{|S_1 = 1, S_{1z}\} \otimes |S_2 = 1, S_{2z}\}$  is a natural choice. By using the Clebsch–Gordan coefficients, we may write state  $\rho$  in the product basis. The partially transposed state with respect to the second spin  $\rho^{T_2}$  can be written in a block-diagonal form with two  $1 \times 1$  blocks, two  $2 \times 2$  blocks, and one  $3 \times 3$  block. After diagonalization of each block, one finds that only two eigenvalues of  $\rho^{T_2}$  are possibly negative (the other eigenvalues are always positive or zero) [31]:

$$\mu_1 = \frac{1}{6}(2 - \langle(\mathbf{S}_i \cdot \mathbf{S}_j)^2\rangle), \quad \mu_2 = \frac{1}{3}(\langle\mathbf{S}_i \cdot \mathbf{S}_j\rangle + \langle(\mathbf{S}_i \cdot \mathbf{S}_j)^2\rangle - 1). \quad (7)$$

Moreover,  $\mu_1$  and  $\mu_2$  occur with multiplicities 3 and 1, respectively. Therefore, the negativity is obtained as

$$\mathcal{N}^{(ij)} = \frac{1}{2} \max[0, \langle(\mathbf{S}_i \cdot \mathbf{S}_j)^2\rangle - 2] + \frac{1}{3} \max[0, 1 - \langle\mathbf{S}_i \cdot \mathbf{S}_j\rangle - \langle(\mathbf{S}_i \cdot \mathbf{S}_j)^2\rangle]. \quad (8)$$

We see that for the  $SU(2)$ -invariant state, the negativity is completely determined by two correlators  $\langle\mathbf{S}_i \cdot \mathbf{S}_j\rangle$  and  $\langle(\mathbf{S}_i \cdot \mathbf{S}_j)^2\rangle$ .

Recall that the swap operator between two spin-1 particles is given by

$$\mathcal{S}_{ij} = \mathbf{S}_i \cdot \mathbf{S}_j + (\mathbf{S}_i \cdot \mathbf{S}_j)^2 - I \quad (9)$$

where  $I$  denotes the  $9 \times 9$  identity matrix. Then, the negativity can be rewritten in the following form:

$$\mathcal{N}^{(ij)} = \frac{1}{2} \max[0, \langle\mathcal{S}_{ij}\rangle - \langle\mathbf{S}_i \cdot \mathbf{S}_j\rangle - 1] + \frac{1}{3} \max[0, -\langle\mathcal{S}_{ij}\rangle]. \quad (10)$$

We see that if the expectation value  $\langle\mathcal{S}_{ij}\rangle < 0$ , the state is entangled. The swap operator satisfies  $\mathcal{S}_{ij}^2 = 1$ , and thus it has only two eigenvalues  $\pm 1$ . If a state is an eigenstate of the swap operator, expression (10) can be simplified. When the corresponding eigenvalue is 1, equation (10) simplifies to

$$\mathcal{N}^{(ij)} = \frac{1}{2} \max[0, -\langle\mathbf{S}_i \cdot \mathbf{S}_j\rangle], \quad (11)$$

and when the eigenvalue is  $-1$ , the equation simplifies to

$$\mathcal{N}^{(ij)} = \frac{1}{3} + \frac{1}{2} \max[0, -\langle\mathbf{S}_i \cdot \mathbf{S}_j\rangle - 2]. \quad (12)$$

In the former case, the state is entangled if  $\langle\mathbf{S}_i \cdot \mathbf{S}_j\rangle < 0$ , and in the latter case, the state is an entangled state, and the negativity is larger than or equal to  $1/3$ .

Now we consider the bilinear–biquadratic spin-1 Heisenberg model described by the Hamiltonian  $H_2$ . By applying the Hellmann–Feynman theorem to the ground state of  $H_2$  and considering the translational invariance, we may obtain the correlators as

$$\langle(\mathbf{S}_i \cdot \mathbf{S}_{i+1})\rangle = \frac{1}{N} \frac{\partial E_{\text{GS}}}{\partial J}, \quad \langle(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2\rangle = \frac{1}{N} \frac{\partial E_{\text{GS}}}{\partial \gamma}, \quad (13)$$

where  $E_{\text{GS}}$  is the ground-state energy. Substituting the above equation into equation (8) yields

$$\mathcal{N}^{(ii+1)} = \frac{1}{2} \max \left[ 0, \frac{1}{N} \frac{\partial E_{\text{GS}}}{\partial \gamma} - 2 \right] + \frac{1}{3} \max \left[ 0, 1 - \frac{1}{N} \frac{\partial E_{\text{GS}}}{\partial J} - \frac{1}{N} \frac{\partial E_{\text{GS}}}{\partial \gamma} \right]. \quad (14)$$

For the case of finite temperature, we have

$$\mathcal{N}^{(ii+1)} = \frac{1}{2} \max \left[ 0, \frac{-1}{N\beta Z} \frac{\partial Z}{\partial \gamma} - 2 \right] + \frac{1}{3} \max \left[ 0, 1 + \frac{1}{N\beta Z} \frac{\partial Z}{\partial J} + \frac{1}{N\beta Z} \frac{\partial Z}{\partial \gamma} \right]. \quad (15)$$

We see that the knowledge of ground-state energy (the partition function) is sufficient to determine the negativity for the case of zero (finite) temperature.

### 3. The bilinear Heisenberg model

Let us now consider entanglement in the bilinear Heisenberg model. Due to the nearest-neighbour character of the interaction, the entanglement between two nearest-neighbour spins is prominent compared with two non-nearest-neighbour spins [15]. Thus, we focus on the nearest-neighbour case in the following discussions of entanglement.

#### 3.1. Two spins

For systems with few spins, we aim at obtaining analytical results of negativity. The Hamiltonian for two spins can be written as

$$H_1 = \mathbf{S}_1 \cdot \mathbf{S}_2 = \frac{1}{2}[(\mathbf{S}_1 + \mathbf{S}_2)^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2], \quad (16)$$

from which all the eigenvalues of the system are given by

$$E_0 = -2(1), \quad E_1 = -1(3), \quad E_2 = 1(5), \quad (17)$$

where the number in the brackets denotes the degeneracy.

We investigate the entanglement of all eigenstates of the system. When the energy level of our system is non-degenerate, the corresponding eigenstate is pure. When a  $k$ th energy level is degenerate, we assume that the corresponding state is an equal mixture of all eigenstates with energy  $E_k$ . Thus, the state corresponding to the  $k$ th level with degeneracy becomes a mixed rather than pure state, keeping all symmetries of the Hamiltonian. This assumption is based on the following fact. An equal mixture of degenerate ground states can be obtained from the thermal state  $\exp[-H/(k_B T)]/Z$  by taking the zero-temperature limit, and the state is called thermal ground state [15]. The  $k$ th eigenstate  $\rho_k$  can be considered as the thermal ground state of the nonlinear Hamiltonian  $H'$  given by  $H' = (H - E_k)^2$ . Note that Hamiltonian  $H'$  inherits all symmetries of Hamiltonian  $H$ .

From equations (8) and (16), we obtain another form of the negativity as

$$\mathcal{N}^{(12)} = \frac{1}{2} \max[0, \langle H_1^2 \rangle - 2] + \frac{1}{3} \max[0, 1 - \langle H_1 + H_1^2 \rangle]. \quad (18)$$

To determine the negativity, it is sufficient to know the cumulants  $\langle H_1 \rangle$  and  $\langle H_1^2 \rangle$ .

From equations (17) and (18), the negativities corresponding to the  $k$ th level are obtained as

$$\mathcal{N}_0^{(12)} = 1, \quad \mathcal{N}_1^{(12)} = 1/3, \quad \mathcal{N}_2^{(12)} = 0. \quad (19)$$

We see that the ground state is a maximally entangled state, the first-excited state is also entangled, but the negativity of the second-excited state is zero.

Having known negativities of all eigenstates, we next consider the case of finite temperature. The cumulants can be obtained from the partition function. From equation (17), the partition function reads

$$Z = e^{2\beta} + 3e^\beta + 5e^{-\beta}. \quad (20)$$

A cumulant of an arbitrary order can be calculated from the partition function as

$$\begin{aligned} \langle H_1^n \rangle &= \frac{(-1)^n}{Z} \frac{\partial^n}{\partial \beta^n} Z \\ &= \frac{(-1)^n}{Z} [2^n e^{2\beta} + 3e^\beta + 5(-1)^n e^{-\beta}]. \end{aligned} \quad (21)$$

Substituting the cumulants with  $n = 1, 2$  into equation (18) yields

$$\mathcal{N} = \frac{1}{2Z} \max(0, 2e^{2\beta} - 3e^\beta - 5e^{-\beta}) + \frac{1}{3Z} \max(0, 3e^\beta - e^{2\beta} - 5e^{-\beta}). \quad (22)$$

Thus, we obtain the analytical expression of the negativity.

The second term in equation (22) can be shown to be zero. To see this fact, it is sufficient to show that  $F(x) = x^3 - 3x^2 + 5 > 0$ , where  $x = e^\beta > 1$ . It is straightforward to check that the function  $F$  takes its minimum 1 at  $x = 2$ . As the minimum is larger than zero, the function is positive definite. Thus, equation (22) simplifies to

$$\mathcal{N} = \frac{1}{2Z} \max(0, 2e^{2\beta} - 3e^\beta - 5e^{-\beta}). \quad (23)$$

The behaviour of the negativity versus temperature is similar to that of the concurrence [43] in the spin-1/2 Heisenberg model [7], namely, the negativity decreases as the temperature increases, and there exists a threshold value of temperature  $T_{\text{th}}$ , after which the negativity vanishes. This behaviour is easy to understand as the increase of temperature leads to the increase of probability of the excited states in the thermal state, and the excited states are less entangled in comparison with the ground state. From equation (23), the threshold temperature can be analytically obtained as

$$T_{\text{th}} = \frac{1}{\ln\left(\frac{1}{2} + \frac{1}{2(11+2\sqrt{30})^{1/3}} + \frac{(11+2\sqrt{30})^{1/3}}{2}\right)} \approx 1.3667. \quad (24)$$

### 3.2. Three spins

The Hamiltonian for three spins can be rewritten as

$$H_1 = \frac{1}{2}[(\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3)^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2 - \mathbf{S}_3^2], \quad (25)$$

from which the ground-state energy and the correlator  $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$  are immediately obtained as

$$E_{\text{GS}} = -3, \quad \langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = -1. \quad (26)$$

In order to know the ground-state negativity, we need to calculate another correlator  $\langle (\mathbf{S}_1 \cdot \mathbf{S}_2)^2 \rangle$ .

By considering the translational invariance and using similar techniques given by [44–46], the ground-state vector is obtained as

$$|\Psi\rangle_{\text{GS}} = \frac{1}{\sqrt{6}}(|012\rangle + |201\rangle + |120\rangle - |021\rangle - |102\rangle - |210\rangle), \quad (27)$$

where  $|n\rangle$  denote the state  $|s = 1, m = s - n\rangle$ , the common eigenstate of  $\mathbf{S}^2$  and  $S_z$ . Then, we can check that

$$\mathbf{S}_1 \cdot \mathbf{S}_2 |\Psi\rangle_{\text{GS}} = -|\Psi\rangle_{\text{GS}}. \quad (28)$$

Thus, the correlator  $\langle (\mathbf{S}_1 \cdot \mathbf{S}_2)^2 \rangle$  is found to be

$$\langle (\mathbf{S}_1 \cdot \mathbf{S}_2)^2 \rangle = 1. \quad (29)$$

Substituting equations (26) and (29) into equation (8) yields

$$\mathcal{N} = 1/3. \quad (30)$$

We see that spins 1 and 2 are in an entangled state at zero temperature. With the increase of temperature, the negativity monotonically decreases until it reaches the threshold value  $T_{\text{th}} = 0.9085$ , after which the negativity vanishes.

### 3.3. Four spins

Now we consider the 4-spin case, and the corresponding Hamiltonian can be written as

$$H_1 = \frac{1}{2}[(\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3 + \mathbf{S}_4)^2 - (\mathbf{S}_1 + \mathbf{S}_3)^2 - (\mathbf{S}_2 + \mathbf{S}_4)^2]. \quad (31)$$

The standard angular momentum coupling theory directly yields the ground-state energy and the correlator  $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ ,

$$E_{\text{GS}} = -6, \quad \langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = -3/2. \quad (32)$$

Then, we need to compute another correlator  $\langle (\mathbf{S}_1 \cdot \mathbf{S}_2)^2 \rangle$  or alternatively the expectation value  $\langle \mathcal{S}_{12} \rangle$ . So, it is necessary to know the exact form of the ground state.

By using similar techniques given by [44–46], the ground-state vector is obtained as

$$|\Psi\rangle_{\text{GS}} = 1/2|\psi_1\rangle - 3/2|\psi_2\rangle + |\psi_3\rangle - 3/2|\psi_4\rangle + 3/\sqrt{2}|\psi_5\rangle + |\psi_6\rangle. \quad (33)$$

where

$$\begin{aligned} |\psi_1\rangle &= 1/2(|0022\rangle + |2002\rangle + |2200\rangle + |0220\rangle), \\ |\psi_2\rangle &= 1/2(|0112\rangle + |2011\rangle + |1201\rangle + |1120\rangle), \\ |\psi_3\rangle &= 1/2(|0121\rangle + |1012\rangle + |2101\rangle + |1210\rangle), \\ |\psi_4\rangle &= 1/2(|0211\rangle + |1021\rangle + |1102\rangle + |2110\rangle), \\ |\psi_5\rangle &= 1/\sqrt{2}(|0202\rangle + |2020\rangle), \\ |\psi_6\rangle &= |1111\rangle. \end{aligned} \quad (34)$$

Then, from the explicit form of the ground state, after two-page calculations, we obtain the expectation value of the swap operator as

$$\langle \mathcal{S}_{12} \rangle = 1/6. \quad (35)$$

Substituting equations (32) and (35) into equation (10) leads to

$$\mathcal{N} = 1/3. \quad (36)$$

It is interesting to see that the ground-state negativity in the 4-qubit model is the same as that in the 3-qubit model. The threshold value is found to be  $T_{\text{th}} = 1.3804$ .

For  $N \geq 5$ , it is hard to obtain analytical results of negativity. The behaviours of negativity are similar to those for  $N \leq 4$ , namely, with the increase of temperature, the negativity decreases until it vanishes at threshold temperature  $T_{\text{th}}$ ; for instance, the threshold temperatures  $T_{\text{th}} \approx 0.95$  and  $T_{\text{th}} \approx 1.21$  for five and six spins, respectively. The negativity for two nearest-neighbours spins is estimated as  $\mathcal{N} = 0.1240$  ( $\mathcal{N} = 0.2509$ ) for the case of five spins (six spins).

Here, we make a comparison of entanglement properties between spin-1/2 and spin-1 systems. For 2- and 4-spin systems, the behaviour of the negativity for the case of spin-1 is similar to that of the concurrence for the case of spin-1/2, namely, with the increase of temperature, both the negativity and the concurrence decrease until they reach zero at certain threshold temperatures. However, for 3-spin systems, there exists a striking difference. The ground state is entangled (not entangled) for the spin-1 (spin-1/2) case [9]. The difference arises from the degeneracy of ground states, which suppresses the entanglement to zero in the spin-1/2 system. It is known that the ground state is non-degenerate for spin-1 Heisenberg chains with any number of spins, and is degenerate for odd-number spin-1/2 chains. Normally, the degeneracy will suppress entanglement. A common feature is that the ground states of 2-spin systems are maximally entangled states, and another common feature is that with the increase of an even number of spins from 2 to 6, the entanglement decreases [13]. We may expect that in a infinite system, the negativity  $\mathcal{N}_{12}$  is still not zero, similar to the entanglement in spin-1/2 systems [13]. However, how to calculate the negativity in the limit of infinite particles is still challenging.

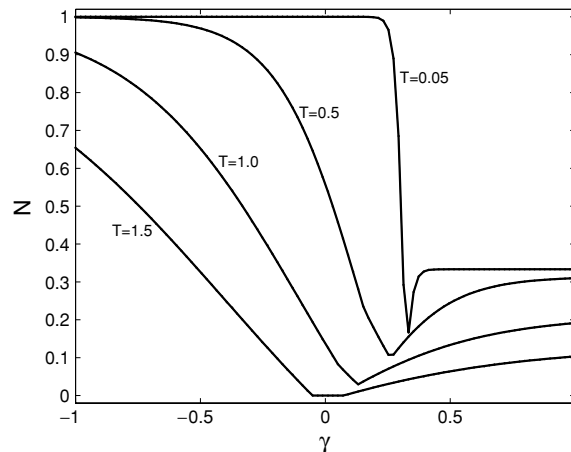


Figure 1. Negativity versus  $\gamma$  for different temperatures in the 2-spin model ( $J = 1$ ).

#### 4. Bilinear–biquadratic spin-1 Heisenberg chains

We now study entanglement properties in the bilinear–biquadratic spin-1 Heisenberg model, and first consider the case of two spins. From equation (14) with  $N = 1$ , if we know the ground-state energy, the negativity is readily obtained. The ground-state energy is given by

$$E_{\text{GS}} = \begin{cases} -2J + 4\gamma & \text{when } \gamma < 1/3, \\ -1J + \gamma & \text{when } \gamma > 1/3. \end{cases} \quad (37)$$

We see that there exists a level crossing at the point of  $\gamma = 1/3$ . Then, substituting the above equation into equation (14) yields

$$\mathcal{N} = \begin{cases} 1 & \text{when } \gamma < 1/3, \\ 1/3 & \text{when } \gamma > 1/3. \end{cases} \quad (38)$$

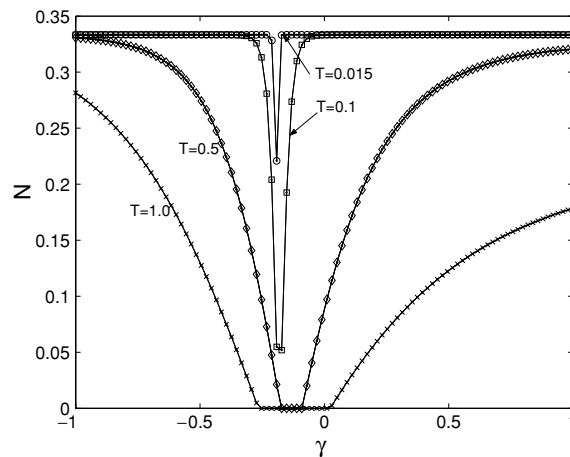
Before the point  $\gamma = 1/3$ , the negativity of the ground-state is 1, while the negativity of the first-excited state is  $1/3$ . After the cross point, the ground and first-excited states interchange, and thus, the negativity of the ground state after the cross point is  $1/3$ . It is interesting to see that the model at the cross point is just the AKLT model.

In figure 1 we plot the negativity versus  $\gamma$  for different temperatures. The level cross greatly affects the behaviours of the negativity at finite temperatures. For a small temperature ( $T = 0.05$ ), the negativity displays a jump to a lower value near the cross point. For higher temperatures, the negativity first decreases, and then increases at  $\gamma$  from  $-1$  to  $1$ . For  $T = 1.5$ , we observe that there exists a range of  $\gamma$  in which the negativity is zero.

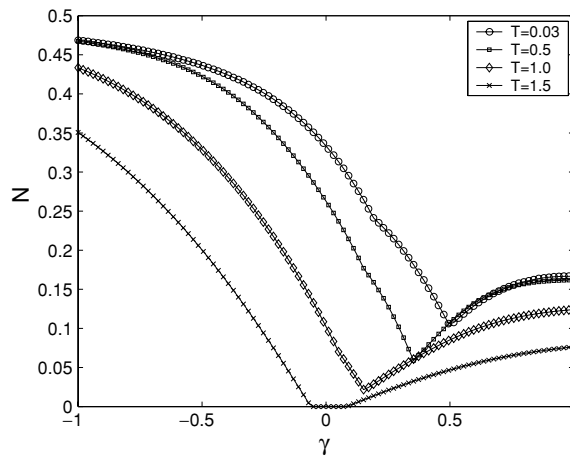
For the 3-spin case, we plot the negativity versus  $\gamma$  for different temperatures in figure 2. For a low temperature  $T = 0.015$ , we observe a dip, which results from the level crossing near the point of  $\gamma = -0.2121$ . When  $T = 0.1$ , the dip becomes more evident. For the cases of higher temperatures ( $T = 0.5$  and  $T = 1.0$ ), there exists a range of parameter  $\gamma$  values, in which the negativity is zero. For the 4-spin case (see figure 3), we also give a plot of the negativity for different temperatures. For  $T = 0.03$ , as  $\gamma$  increases, the negativity decreases until it reaches its minimum, and then increases. For  $T = 0.5$  and  $1.0$ , the behaviours of negativity are similar to the case of  $T = 0.01$ , and the difference is that the minima shift left.

Comparing cases with different  $N$ , we observe some common features in the behaviours of negativity. (1) The maximum value of negativity occurs at  $\gamma = -1$ ; (2) for higher





**Figure 2.** Negativity versus  $\gamma$  for different temperatures in the 3-spin model ( $J = 1$ ).



**Figure 3.** Negativity versus  $\gamma$  for different temperatures in the 4-spin model ( $J = 1$ ).

temperatures, there exists a range of  $\gamma$ , in which the negativity is zero; and (3) for lower temperatures, the minimum value occurs at a certain value of  $\gamma$ . The first feature is due to the fact that the biquadratic term with  $\gamma = -1$  leads the system to be in the maximally entangled state (the anti-ferromagnetic case). The second and third features result from the competition between the bilinear and biquadratic terms in the Hamiltonian.

We numerically calculated the threshold temperature and the results are shown in figure 4. The threshold temperature decreases nearly linearly when  $\gamma$  increases from  $-1$  to a certain value of  $\gamma$ . After reaching a minimum, it begins to increase. We see that the behaviours of the threshold temperature are similar for the different numbers of spins. The maximum value of the threshold temperature occurs at  $\gamma = -1$ . This is also due to the fact that the biquadratic term with  $\gamma = -1$  leads the system to be in the maximally entangled state. The higher the negativity at zero temperature, the higher the threshold temperature.

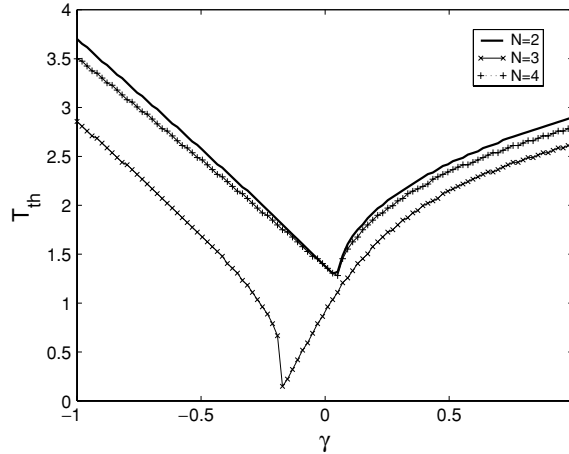


Figure 4. Threshold temperature versus  $\gamma$  for different numbers of spins.

As a final remark, we consider the following Hamiltonian,

$$H_3 = \sum_{i \neq j}^N J \mathbf{S}_i \cdot \mathbf{S}_j = \frac{1}{2} \left( \sum_{i=1}^N \mathbf{S}_i \right)^2 - N, \quad (39)$$

where the interaction is between all spins, and there are altogether  $N(N-1)/2$  terms. The system not only shows an  $SU(2)$  symmetry, but also an exchange symmetry, namely, the Hamiltonian is invariant under exchange operation  $S_{ij} H_3 S_{ij} = H_3$ . For  $N = 2, 3$ , the model is identical to Hamiltonian  $H_1$ . We know that the ground state is non-degenerate when  $N = 2, 3$ , and thus it must be an eigenstate of  $S_{ij}$  and equations (11) and (12) can apply. From the angular momentum coupling theory, the ground-state energy of  $H_3$  is readily obtained as  $E_{GS} = -N$ , and thus we have  $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle = -2/(N-1)$ . Then, from equations (11) and (12), the negativity can be either  $1/(N-1)$  or  $1/3$ . For  $N = 2(N = 3)$ , the ground state is symmetric (antisymmetric) and then the negativity is  $1$  ( $1/3$ ), consistent with the previous results. However, for  $N \geq 4$ , the ground state is degenerate and we cannot apply equations (11) and (12). The numerical results show that the negativity is zero for  $N \geq 4$ .

## 5. Conclusions

In conclusion, by using the concept of negativity, we have studied entanglement in spin-1 Heisenberg chains. Both the bilinear model and bilinear–biquadratic model are considered. We have given explicitly the relation between the negativity and two correlators. The merit of this relation is that the two correlators completely determine the negativity and it facilitates our discussions of entanglement properties.

We have obtained analytical results of negativity in the bilinear model up to four spins and in the 2-spin bilinear–biquadratic model. We numerically calculated entanglement in the bilinear–biquadratic model for  $N = 2, 3, 4$ , and the threshold temperatures versus  $\gamma$  are also given. We have restricted us to the small-size systems, and aimed at obtaining analytical results via symmetry considerations and getting some numerical results via the exact diagonalization method. However, for larger systems, the exact diagonalization method is not a viable route.

It is interesting to investigate large systems by some mature numerical methods such as the quantum Monte Carlo method and density-matrix renormalization group method. It is also interesting to consider other  $SU(2)$ -invariant spin-1 systems such as the dimerized and frustrated systems.

### Acknowledgments

We thank G M Zhang, C P Sun and Z Song for helpful discussions. This work is supported by the National Natural Science Foundation of China under grant no 10405019.

### References

- [1] Haldane F D M 1983 *Phys. Lett. A* **93** 464  
Haldane F D M 1983 *Phys. Rev. Lett.* **50** 1153
- [2] Affleck I, Kennedy T, Lieb E H and Tasaki H 1987 *Phys. Rev. Lett.* **59** 799
- [3] Millet P, Mila F, Zhang F C, Mambrini M, Van Oosten A B, Pashchenko V A, Sulpice A and Stepanov A 1999 *Phys. Rev. Lett.* **83** 4176
- [4] Lou J Z, Xiang T and Su Z B 2000 *Phys. Rev. Lett.* **85** 2380
- [5] Schollwöck, Jolicoeur T and Garel T 1996 *Phys. Rev. B* **53** 3304
- [6] Nielsen M A 1998 *PhD Thesis* University of Mexico *Preprint* quant-ph/0011036
- [7] Arnesen M C, Bose S and Vedral V 2001 *Phys. Rev. Lett.* **87** 017901
- [8] Gunlycke D, Kendon V M, Vedral V and Bose S 2001 *Phys. Rev. A* **64** 042302
- [9] Wang X 2001 *Phys. Rev. A* **64** 012313  
Wang X 2001 *Phys. Lett. A* **281** 101  
Wang X and Zanardi P 2002 *Phys. Lett. A* **301** 1  
Wang X 2002 *Phys. Rev. A* **66** 044305  
Wang X, Fu H and Solomon A I 2001 *J. Phys. A: Math. Gen.* **34** 11307  
Wang X and Mölmer K 2002 *Eur. Phys. J. D* **18** 385
- [10] Jaeger G, Sergienko A V, Saleh B E A and Teich M C 2003 *Phys. Rev. A* **68** 022318
- [11] Bose S and Vedral V 2000 *Phys. Rev. A* **61** 040101
- [12] Kamta G L and Starace A F 2002 *Phys. Rev. Lett.* **88** 107901
- [13] O'Connor K M and Wootters W K 2001 *Phys. Rev. A* **63** 0520302
- [14] Meyer D A and Wallach N R 2001 *Preprint* quant-ph/0108104
- [15] Osborne T J and Nielsen M A 2002 *Phys. Rev. A* **66** 032110
- [16] Osterloh A, Amico L, Falci G and Fazio R 2002 *Nature* **416** 608
- [17] Sun Y, Chen Y G and Chen H 2003 *Phys. Rev. A* **68** 044301
- [18] Glaser U, Büttner H and Fehske H 2003 *Phys. Rev. A* **68** 032318
- [19] Santos L F 2003 *Phys. Rev. A* **67** 062306
- [20] Yeo Y 2002 *Phys. Rev. A* **66** 062312
- [21] Khveshchenko D V 2003 *Phys. Rev. B* **68** 193307
- [22] Zhou L, Song H S, Guo Y Q and Li C 2003 *Phys. Rev. A* **68** 024301
- [23] Brennen G K and Bullock S S 2004 *Phys. Rev. A* **70** 52303
- [24] Xin R, Song Z and Sun C P 2005 *Phys. Lett. A* **342** 30
- [25] Tóth G 2005 *Phys. Rev. A* **71** 010301
- [26] Verstraete F, Popp M and Cirac J I 2004 *Phys. Rev. Lett.* **92** 027901
- [27] Verstraete F, Martin-Delgado M A and Cirac J I 2004 *Phys. Rev. Lett.* **92** 087201
- [28] Vidal J, Palacios G and Mosseri R 2004 *Phys. Rev. A* **69** 022107
- [29] Lambert N, Emary C and Brandes T 2004 *Phys. Rev. Lett.* **92** 073602
- [30] Ghose S, Rosenbaum T F, Aeppli G and Coppersmith S N 2003 *Nature* **425** 48
- [31] Schliemann J 2003 *Phys. Rev. A* **68** 012309
- [32] Brukner C, Vedral V and Zeilinger A *Preprint* quant-ph/0410138  
Brukner C and Vedral V 2004 *Preprint* quant-ph/0406040
- [33] Fan H, Korepin V and Roychowdhury V 2004 *Phys. Rev. Lett.* **93** 227203
- [34] Verstraete F, Martin-Delgado M A and Cirac J I 2004 *Phys. Rev. Lett.* **92** 087201
- [35] Zhou L, Yi X X, Song H S and Quo Y Q 2005 *Chinese Phys.* **14** 1168
- [36] Gu S J, Lin H Q and Li Y Q 2003 *Phys. Rev. A* **68** 042330

- 
- [37] Wang X 2004 *Phys. Rev. E* **69** 066118  
Wang X 2004 *Phys. Lett. A* **329** 439  
Wang X 2005 *Phys. Lett. A* **334** 352
- [38] Chen Y, Zanardi P, Wang Z D and Zhang F C 2004 *Preprint* quant-ph/0407228
- [39] Vidal G, Latorre J I, Rico E and Kitaev A 2003 *Phys. Rev. Lett.* **90** 227902
- [40] Bennett C H, Brassard G, Crepeau C, Jozsa R, Peres A and Wootters W K 1993 *Phys. Rev. Lett.* **70** 1895
- [41] Vidal G and Werner R F 2002 *Phys. Rev. A* **65** 032314
- [42] Peres A 1996 *Phys. Rev. Lett.* **77** 1413  
Horodecki M, Horodecki P and Horodecki R 1996 *Phys. Lett. A* **223** 1
- [43] Wootters W K 1998 *Phys. Rev. Lett.* **80** 2245
- [44] Kouzoudis D 1997 *J. Magn. Magn. Mater.* **173** 259  
Kouzoudis D 1998 *J. Magn. Magn. Mater.* **189** 366
- [45] Bärwinkel K, Schmidt H-J and Schnack J 2000 *J. Magn. Magn. Mater.* **220** 227
- [46] Lin H Q 1990 *Phys. Rev. B* **42** 6561