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Negativity, entanglement witness and quantum phase transition in spin-1 Heisenberg chains

Xiaoguang Wang[1,2] **and Shi-Jian Gu**[1]

[1] Department of Physics and Institute of Theoretical Physics, The Chinese University of Hong Kong, Hong Kong, People's Republic of China
[2] Zhejiang Institute of Modern Physics, Department of Physics, Zhejiang University, HangZhou 310027, People's Republic of China

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Abstract
We propose to use negativity and entanglement witnesses to study quantum phase transitions in the bilinear–biquadratic and anisotropic *XXZ* spin-1 models. We obtain an analytical expression of negativity in the *XXZ* model and an entanglement witness. The roles of the negativity and entanglement witnesses in the quantum phase transitions in these two models are studied numerically.

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1. Introduction

In the past two decades, various kinds of properties of spin chains have been studied. Specifically, spin-1 chains attract more attention since Haldane predicts that the one-dimensional Heisenberg chain has a spin gap for integer spins [1]. In these studies, the bilinear–biquadratic (BB) Heisenberg model and the anisotropic spin-1 *XXZ* model have played important roles [2–5], and the corresponding Hamiltonians are given by

$$H_{\mathrm{BB}} = \sum_{i=1}^{N} \cos\theta(\mathbf{s}_i \cdot \mathbf{s}_{i+1}) + \sin\theta(\mathbf{s}_i \cdot \mathbf{s}_{i+1})^2, \tag{1}$$

$$H_{XXZ} = \sum_{i=1}^{N} (s_{ix}s_{i+1x} + s_{iy}s_{i+1y} + \Delta s_{iz}s_{i+1z}), \tag{2}$$

respectively. Here, $\mathbf{s}_i$ denotes the spin-1 operator at site i, Δ characterizes the anisotropy of the model, and we assume the periodic boundary conditions. The first Hamiltonian exhibits a SU(2) symmetry, and displays a very rich quantum phase diagram [6]. For the second model, it was found that between the ground-state gapless XY phase and the doublet antiferromagnetic

(AF) phase, there exists a new phase characterized by a nonmagnetic singlet state over an extended range of Δ values ($0.61 \lesssim \Delta \lesssim 1.18$) [5, 7–9]. This is completely different from that in the spin-1/2 *XXZ* model.

The study of quantum phase transition (QPT) occurred at zero temperature is very challenging, and there exist different approaches. Recent studies reveal that the quantum entanglement can be an efficient indicator of QPT [11, 10]. Quantum entanglement lies at the heart of quantum mechanics, and can be exploited to accomplish some physical tasks such as quantum teleportation. 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 studied less. There are several proceeding works on entanglement in spin-1 chains. Fan *et al* [12] and Verstraete *et al* [13] studied entanglement in the bilinear–biquadratic model with a special value of θ, i.e., the AKLT model [2]. Zhou *et al* studied entanglement in a spin dimer [14]. Gu *et al* [15] and Legaza *et al* [16] calculated the two-site entropy in spin-1 systems.

We study pairwise entanglement of two spins in spin-1 many-body systems. The two spins are in a mixed state after tracing out other spins. For mixed-state entanglement of two spin ones, there are no operational entanglement criteria until now. However, we still can use the Peres–Horodecki criterion which gives a qualitative way for judging if a state is entangled [17]. It is well known that it cannot detect bound entanglement in higher-dimension systems. For states with certain symmetries, this criterion is good enough to characterize entanglement [18, 19]. The quantitative version of the criterion was developed by Vidal and Werner [20]. They presented a measure of entanglement called negativity. The negativity of a two-spin state ρ is defined as

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

where μ_i is the negative eigenvalue of ρ^{T_2}, and T_2 denotes the partial transpose (PT) with respect to the second system. If $\mathcal{N} > 0$, then the two-spin state is entangled.

In addition to negativity, the entanglement witness (EW) [21] is also considered. Entanglement witnesses are physical observables which are closely related to negativity, and may be used to signify QPT points. An entanglement witness is an observable W which satisfies $\mathrm{Tr}(W\rho_{\mathrm{sep}})$ for all separable states ρ_{sep}, and $\mathrm{Tr}(W\rho) < 0$ for at least one entangled state ρ.

We organized our paper as follows: In section 2, we give the negativity expression for the bilinear–biquadratic system, and derive the negativity for the *XXZ* system and give a new entanglement witness operator. In section 3, we give numerical results of negativity and entanglement witnesses, and discuss relations with QPTs. Conclusion is given in section 4.

2. General expression of negativity

We now give the negativity expressions in the above two spin-1 models.

2.1. The bilinear–biquadratic model

The BB Hamiltonian is SU(2)-invariant, so does the thermal state $\rho_T = \mathrm{e}^{-\beta H}/Z$. Here, $\beta = 1/T$, the Boltzmann constant is set to be one, and Z is the partition function. The ground state is obtained from the thermal state by taking the zero-temperature limit. This kind of ground state was referred to thermal ground state [11], and has the benefit that it is

SU(2)-invariant (no symmetry breaking). For SU(2)-invariant state, the expression of the negativity for spin pair i and j is given by [18, 19, 22]

$$\mathcal{N}_{ij} = \tfrac{1}{3}\max[0, 1 - \langle \mathbf{s}_i \cdot \mathbf{s}_j\rangle - \langle(\mathbf{s}_i \cdot \mathbf{s}_j)^2\rangle] + \tfrac{1}{2}\max[0, \langle(\mathbf{s}_i \cdot \mathbf{s}_j)^2\rangle - 2]. \tag{4}$$

We see that the negativity is completely determined by two correlators $\langle \mathbf{s}_i \cdot \mathbf{s}_j\rangle$ and $\langle(\mathbf{s}_i \cdot \mathbf{s}_j)^2\rangle$. By using the swap operator and the singlet projector given by

$$\mathbf{S}_{ij} = \mathbf{s}_i \cdot \mathbf{s}_j + (\mathbf{s}_i \cdot \mathbf{s}_j)^2 - \mathbf{1} \tag{5}$$

$$\mathbf{P}_{ij} = \tfrac{1}{3}[(\mathbf{s}_i \cdot \mathbf{s}_j)^2 - \mathbf{1}], \tag{6}$$

we reexpress the negativity as

$$\mathcal{N}_{ij} = \tfrac{1}{3}\max[0, -\langle \mathbf{S}_{ij}\rangle] + \tfrac{1}{2}\max[0, \langle 3\mathbf{P}_{ij} - 1\rangle]. \tag{7}$$

From this expression, it is evident that there are two entanglement witnesses

$$W_1 = \mathbf{S}_{ij}, \tag{8}$$

$$W_2 = 1 - 3\mathbf{P}_{ij}. \tag{9}$$

Indeed, the negativity is closely related to EWs, and by studying negativity, one may find some useful entanglement witnesses. Moreover, we give another form of the negativity

$$\begin{aligned}\mathcal{N}_{ij} = \tfrac{3}{2}\max\left[0, \left\langle \mathbf{s}_z^2 \otimes \mathbf{s}_z^2 + 2\mathbf{s}_x\mathbf{s}_y \otimes \mathbf{s}_y\mathbf{s}_x\right\rangle - \tfrac{2}{3}\right] \\ + \max\left[0, \tfrac{1}{3} - \left\langle \mathbf{s}_z \otimes \mathbf{s}_z + \mathbf{s}_z^2 \otimes \mathbf{s}_z^2 + 2\mathbf{s}_x\mathbf{s}_y \otimes \mathbf{s}_y\mathbf{s}_x\right\rangle\right],\end{aligned} \tag{10}$$

following from the SU(2) symmetry.

2.2. The XXZ model

When studying negativity in the *XXZ* model, we can make use of the symmetries in the model to simplify the negativity expression. Due to the U(1) symmetry ($[\mathrm{e}^{-\mathrm{i}\theta \mathbf{J}_z}, H] = 0, \mathbf{J}_\alpha = \sum_{i=1}^N \mathbf{s}_{i\alpha}, \alpha = x, y, z.$), in the basis $\{|02\rangle, |11\rangle, |20\rangle, |01\rangle, |10\rangle, |12\rangle, |21\rangle, |00\rangle, |22\rangle\}$, the reduced density matrix of two spins can always be written in a block diagonal form as

$$\rho_{ij} = \mathrm{diag}(A_{3\times 3}, B_{2\times 2}, C_{2\times 2}, a_8, a_9) \tag{11}$$

with A, B and C given by

$$A = \begin{pmatrix} a_1 & b_1 & b_2 \\ b_1 & a_2 & b_3 \\ b_2 & b_3 & a_3 \end{pmatrix}, \qquad B = \begin{pmatrix} a_4 & b_4 \\ b_4 & a_5 \end{pmatrix}, \qquad C = \begin{pmatrix} a_6 & b_5 \\ b_5 & a_7 \end{pmatrix}. \tag{12}$$

Here, state $|n\rangle \equiv |j = 1, m = 1 - n\rangle$ for one spin.

For the diagonal elements, we have

$$a_1 = a_3, \qquad a_8 = a_9, \qquad a_4 = a_5 = a_6 = a_7. \tag{13}$$

As an example, we prove the first equality, and the others can be similarly proved. For one spin, the following relations exist:

$$\begin{aligned} &|0\rangle\langle 0| - |2\rangle\langle 2| = \mathbf{s}_z, \qquad |0\rangle\langle 0| + |2\rangle\langle 2| = \mathbf{s}_z^2 \\ &|0\rangle\langle 0| + |1\rangle\langle 1| + |2\rangle\langle 2| = \mathbf{1}. \end{aligned} \tag{14}$$

From the above equation, one can write the three projectors in terms of operators $\mathbf{s}_z$ and $\mathbf{s}_z^2$ as

$$|0\rangle\langle 0| = \frac{\mathbf{s}_z^2 + \mathbf{s}_z}{2}, \qquad |1\rangle\langle 1| = \mathbf{1} - \mathbf{s}_z^2, \qquad |2\rangle\langle 2| = \frac{\mathbf{s}_z^2 - \mathbf{s}_z}{2}. \tag{15}$$

The diagonal elements a_1 and a_3 can be written as the expectation values of the following operators

$$
\begin{aligned}
|0\rangle\langle 0| \otimes |2\rangle\langle 2| &= \tfrac{1}{4}\left(\mathbf{s}_z^2 \otimes \mathbf{s}_z^2 - \mathbf{s}_z \otimes \mathbf{s}_z - \mathbf{s}_z^2 \otimes \mathbf{s}_z + \mathbf{s}_z \otimes \mathbf{s}_z^2\right) \\
|2\rangle\langle 2| \otimes |0\rangle\langle 0| &= \tfrac{1}{4}\left(\mathbf{s}_z^2 \otimes \mathbf{s}_z^2 - \mathbf{s}_z \otimes \mathbf{s}_z + \mathbf{s}_z^2 \otimes \mathbf{s}_z - \mathbf{s}_z \otimes \mathbf{s}_z^2\right),
\end{aligned} \tag{16}
$$

respectively. Due to another symmetry $[\mathrm{e}^{-\mathrm{i}\pi \mathbf{J}_x}, H] = [\mathrm{e}^{-\mathrm{i}\pi \mathbf{J}_y}, H] = 0$, one can easily show that the expectation values of $\mathbf{s}_z^2 \otimes \mathbf{s}_z$ and $\mathbf{s}_z \otimes \mathbf{s}_z^2$ are zero. Thus, we finally obtain $a_1 = a_3$. Similarly, we have $a_4 = a_7, a_5 = a_6$. Then, after using the translational invariant symmetry of the Hamiltonian, finally we get $a_4 = a_5 = a_6 = a_7$.

Again, due to $[\mathrm{e}^{-\mathrm{i}\pi \mathbf{J}_x}, H] = 0$, we obtain

$$
\begin{aligned}
a_8 &= \mathrm{Tr}(|0\rangle\langle 0| \otimes |0\rangle\langle 0| \rho_T) \\
&= \mathrm{Tr}(\mathrm{e}^{-\mathrm{i}\pi \mathbf{J}_x} |0\rangle\langle 0| \otimes |0\rangle\langle 0|\, \mathrm{e}^{\mathrm{i}\pi \mathbf{J}_x} \rho_T)
\end{aligned} \tag{17}
$$

$$
\begin{aligned}
&= \mathrm{Tr}(\mathrm{e}^{-\mathrm{i}\pi \mathbf{s}_{1x}} |0\rangle\langle 0|\, \mathrm{e}^{\mathrm{i}\pi \mathbf{s}_{1x}} \otimes \mathrm{e}^{-\mathrm{i}\pi \mathbf{s}_{2x}} |0\rangle\langle 0|\, \mathrm{e}^{\mathrm{i}\pi \mathbf{s}_{2x}} \rho_T) \\
&= \mathrm{Tr}(|2\rangle\langle 2| \otimes |2\rangle\langle 2| \rho_T) = a_9.
\end{aligned} \tag{18}
$$

In the derivation of the above inequality, we have used the results that

$$
\mathrm{e}^{-\mathrm{i}\pi \mathbf{s}_x} |0\rangle = -|2\rangle, \qquad \mathrm{e}^{-\mathrm{i}\pi \mathbf{s}_x} |2\rangle = -|0\rangle, \qquad \mathrm{e}^{-\mathrm{i}\pi \mathbf{s}_x} |1\rangle = -|1\rangle, \tag{19}
$$

and these can be obtained from the following fact:

$$
\mathrm{e}^{-\mathrm{i}\pi \mathbf{s}_x} = \mathbf{1} - 2\mathbf{s}_x^2 = -\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}. \tag{20}
$$

Similarly, for non-diagonal elements, $b_1 = b_3$ and $b_4 = b_5$. Then, the reduced density matrix can now be written in a simplified form as

$$
\rho_{12} = \mathrm{diag}(A_{3\times 3}, B_{2\times 2}, B_{2\times 2}, a_8, a_8) \tag{21}
$$

with A, B and C given by

$$
A = \begin{pmatrix} a_1 & b_1 & b_2 \\ b_1 & a_2 & b_1 \\ b_2 & b_1 & a_1 \end{pmatrix}, \qquad B = \begin{pmatrix} a_4 & b_4 \\ b_4 & a_4 \end{pmatrix}. \tag{22}
$$

Now, we make the PT with respect to the second spin system. After the PT, in the basis spanned by $\{|00\rangle, |11\rangle, |22\rangle, |01\rangle, |12\rangle, |10\rangle, |21\rangle, |02\rangle, |20\rangle\}$, the reduced density matrix can also be written in a block diagonal form as

$$
\rho_{12}^{T_2} = \mathrm{diag}(C_{3\times 3}, D_{2\times 2}, D_{2\times 2}, a_1, a_1) \tag{23}
$$

with C, D given by

$$
C = \begin{pmatrix} a_8 & b_4 & b_2 \\ b_4 & a_2 & b_4 \\ b_2 & b_4 & a_8 \end{pmatrix}, \qquad D = \begin{pmatrix} a_4 & b_1 \\ b_1 & a_4 \end{pmatrix}. \tag{24}
$$

Formally, matrices ρ_{12} and $\rho_{12}^{T_2}$ are connected by the following exchanges $a_1 \leftrightarrow a_8, b_1 \leftrightarrow b_4$.

The matrix C can be further written in a block-diagonal form with one 2×2 block and another 1×1 as

$$
E = \begin{pmatrix} a_8 + b_2 & \sqrt{2} b_4 & 0 \\ \sqrt{2} b_4 & a_2 & 0 \\ 0 & 0 & a_8 - b_2 \end{pmatrix},
$$

in the basis $\left\{\frac{1}{\sqrt{2}}(|02\rangle + |20\rangle), |11\rangle, \frac{1}{\sqrt{2}}(|02\rangle - |20\rangle)\right\}$. Then, it is straightforward to find all nine eigenvalues of the partially transposed matrix, and among them, only the following three eigenvalues are possibly negative

$$\begin{aligned}\lambda_1 &= \tfrac{1}{2}\left[a_8 + b_2 + a_2 - \sqrt{(a_8 + b_2 - a_2)^2 + 8b_4^2}\right],\\ \lambda_2 &= a_8 - b_2,\\ \lambda_3 &= a_4 - |b_1|.\end{aligned} \tag{25}$$

Formally, the negativity can be written as

$$\mathcal{N} = \max[0, -\lambda_1] + \max[0, -\lambda_2] + \max[0, -\lambda_3]. \tag{26}$$

Relevant elements of the reduced density matrix can be written in terms of spin operators as follows

$$\begin{aligned}a_8 &= \tfrac{1}{4}\left\langle \mathbf{s}_z^2 \otimes \mathbf{s}_z^2 + \mathbf{s}_z \otimes \mathbf{s}_z\right\rangle\\ a_4 &= \tfrac{1}{2}\left\langle \mathbf{s}_z^2 \otimes I - \mathbf{s}_z^2 \otimes \mathbf{s}_z^2\right\rangle\\ a_2 &= \left\langle 1 - 2\mathbf{s}_z^2 \otimes I + \mathbf{s}_z^2 \otimes \mathbf{s}_z^2\right\rangle\\ b_2 &= \tfrac{1}{8}\left\langle \mathbf{s}_+^2 \otimes \mathbf{s}_-^2 + \mathbf{s}_-^2 \otimes \mathbf{s}_+^2\right\rangle\\ &= \tfrac{1}{4}\big\langle \left(\mathbf{s}_x^2 - \mathbf{s}_y^2\right) \otimes \left(\mathbf{s}_x^2 - \mathbf{s}_y^2\right)\\ &\quad + (\mathbf{s}_x\mathbf{s}_y + \mathbf{s}_y\mathbf{s}_x) \otimes (\mathbf{s}_x\mathbf{s}_y + \mathbf{s}_y\mathbf{s}_x)\big\rangle\\ b_1 &= -\tfrac{1}{4}\langle \mathbf{s}_z\mathbf{s}_+ \otimes \mathbf{s}_z\mathbf{s}_- + \mathbf{s}_-\mathbf{s}_z \otimes \mathbf{s}_+\mathbf{s}_z\rangle\\ &= -\tfrac{1}{2}\langle \mathbf{s}_z\mathbf{s}_x \otimes \mathbf{s}_z\mathbf{s}_x + \mathbf{s}_x\mathbf{s}_z \otimes \mathbf{s}_x\mathbf{s}_z\rangle\\ b_4 &= \tfrac{1}{4}\langle \mathbf{s}_z\mathbf{s}_+ \otimes \mathbf{s}_-\mathbf{s}_z + \mathbf{s}_-\mathbf{s}_z \otimes \mathbf{s}_z\mathbf{s}_+\rangle\\ &= \tfrac{1}{2}\langle \mathbf{s}_z\mathbf{s}_x \otimes \mathbf{s}_x\mathbf{s}_z + \mathbf{s}_x\mathbf{s}_z \otimes \mathbf{s}_z\mathbf{s}_x\rangle.\end{aligned}$$

Then, as a byproduct, from the above equation and equation (26), one may find that the operator

$$\begin{aligned}W_3 &= a_8 - b_2\\ &= \tfrac{1}{4}\left[\mathbf{s}_z^2 \otimes \mathbf{s}_z^2 + \mathbf{s}_z \otimes \mathbf{s}_z - \tfrac{1}{2}\left(\mathbf{s}_+^2 \otimes \mathbf{s}_-^2 + \mathbf{s}_-^2 \otimes \mathbf{s}_+^2\right)\right]\end{aligned} \tag{27}$$

is an EW which detects entanglement in the *XXZ* model. By considering several symmetries in the model, we have obtained the analytical expression of the negativity, and found a new EW.

3. Numerical results

Next, we provide numerical results of negativity and EWs for the BB and *XXZ* models. The exact-diagonalization method is employed.

3.1. The BB model

In figure 1, we plot the negativity of two nearest spins and ground-state expectation values of EWs versus θ for 12 spins. We observe a maximum of negativity and a minimum of $\langle W_1\rangle$ at $\theta = \pi/4$, which separate the Haldane phase $(-\pi/4 < \theta < \pi/4)$ and the trimerized phase $(\pi/4 < \theta < \pi/2)$. We see that both the negativity and the EW W_1 can detect this QPT point. Before $\theta = \pi/4$, there is a minimum of the negativity, which results from the competition of two EWs. Clearly, this minimum point is singular even for a finite system, and does not correspond to the QPT point.

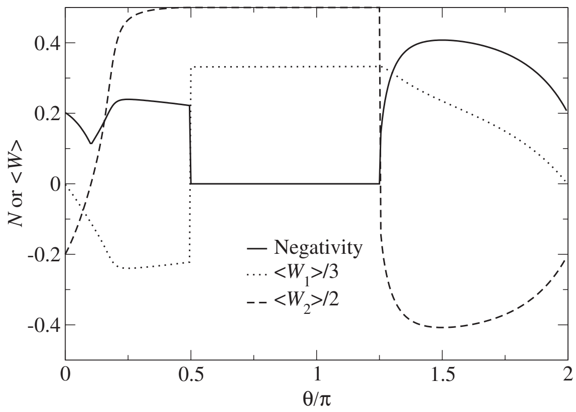

Figure 1. Negativity and ground-state expectation values of EWs versus θ for 12 spins.

For $\pi/2 < \theta < 5\pi/4$, the ground state is ferromagnetic and degenerate. In this range, the negativity is zero. Comparing the pairwise entanglement with bipartite entanglement between the two nearest-neighbor spins and the rest, the pairwise negativity is well defined, while, due to the degeneracy, the bipartite entanglement quantified by the von Neumann entropy is not well defined. This is one of the merits of our approach using negativity.

For $\theta > 5\pi/4$, we observe a maximum of the negativity and a minimum of $\langle W_2\rangle$ at $\theta = 3\pi/2$. Detailed analysis on the energy spectra reveals that the first excited state at this point is eight-fold degenerate, and at one side of this point it is three-fold degenerate, and at another side five-fold degenerate. Then the extremum of the negativity and $\langle W_2\rangle$ is closely related the high symmetry at this point. This phenomenon is very similar to the case of the concurrence at $\Delta = 1$ in spin-1/2 *XXZ* model, [23] so it may be another critical point in the BB model. However, at $\theta = 7\pi/4$, corresponding to a QPT point separating dimerized phase ($5\pi/4 < \theta < 7\pi/4$) and Haldane phase, one cannot find any anomalous behaviors of negativity and EWs.

Due to the nearest-neighbor nature of the interactions, entanglement of the nearest-neighbor pair is larger than that of non-nearest-neighbor pairs. And for spin-1/2 systems, it was found that the entanglement vanishes quickly as the separation distance of two spins increases [11]. Here, for spin-1 system, we find that the entanglement is relatively stable against separation distance for the BB model with $\theta = (1.25\pi)^+$. The numerical result is shown in figure 2. The symmetry in the figure is easily understood due to the periodic boundary condition. It is evident that all pairs of spins are entangled, and, of course, the entanglement decreases as the absolute separation distance increases. This relatively long range feature of negativity is in big contrast with that of concurrence in spin-1/2 systems, and may result from that higher-dimensional nature and special properties of integer-spin systems.

3.2. *The XXZ model*

Let us consider the spin-1 *XXZ* model. At the isotropic point ($\Delta = 0$), the spin excitation spectrum is gapped according to Haldane's conjecture [1]. As Δ increases, this gap vanishes around $\Delta = \Delta_u \approx 1.18$. At this point, the system undergoes a Kosterlitz–Thouless type of phase transition from the gapped phase to gapless Néel phase. The gapped phase extends over the anisotropy parameter ($\Delta_l \leqslant \Delta \leqslant \Delta_u$) including the isotropic point, and Δ_l is estimated

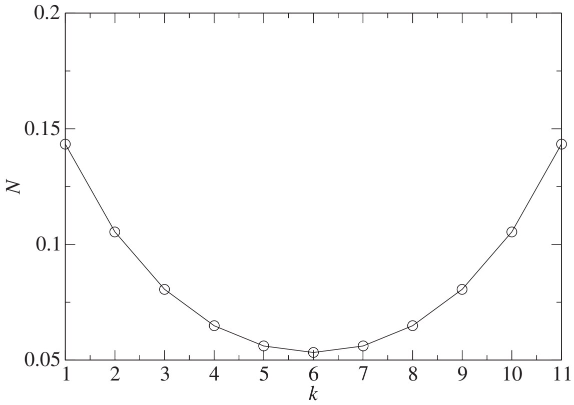

Figure 2. Negativity $\mathcal{N}_{1,1+k}$ versus separation distance k in the BB model with $\theta = (1.25\pi)^+$ for 12 spins.

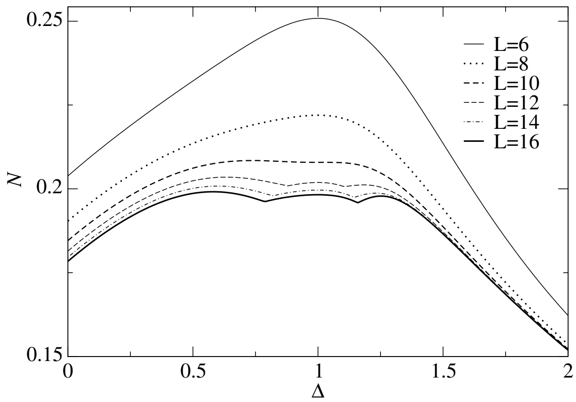

Figure 3. Negativity versus Δ for different number of spins.

to be 0.61 from several independent calculations [7]. The transition from the XY phase to the gapped phase occurs at $\Delta = \Delta_l$. From the two-spin reduced density matrix, we may obtain the von Neumann entropy quantifying the entanglement of the two spin with the rest, and the negativity quantifying the entanglement between the two spins. Both these two quantities can serve as indicators of QPT. It is argued that the two-site entropy is better to indicate QPT than single-site entropy and order parameters [16]. We will see that the negativity is more sensitive to variation parameters than the von Neumann entropy.

In figure 3, we plot the negativity versus Δ. We observe a maximum of negativity at the SU(2) point $\Delta = 1$. Similarly, the von Neumann entropy also displays a maximum at this point [15]. Although it is an extreme point, it does not correspond to a QPT point as the system is gapped on both sides of the point, contrary to the case of spin-1/2 XXZ systems [24].

For the size of our system being large enough, we observe that there are two minima at Δ_1 and Δ_2 beside the SU(2) point. These minima do not happen in the behaviors of the von Neumann entropy, indicating that the negativity is more sensitive to variation of parameters.

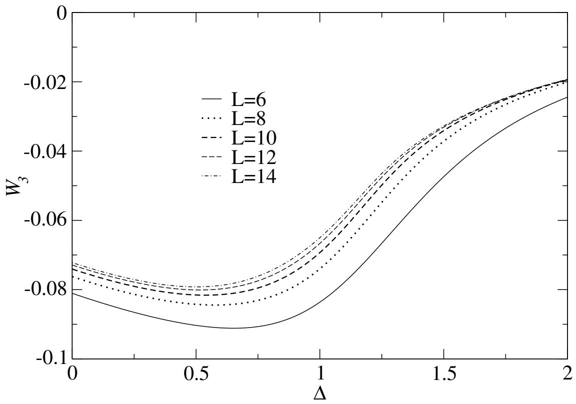

Figure 4. Expectation value of entanglement witness of W_3 versus Δ for different number of spins.

As system size increases, the Δ_1 tends to Δ_l, and the Δ_1 to Δ_u, respectively, supporting that QPT happens at $\Delta = \Delta_u$ and Δ_l.

We have found a entanglement witness W_3 (27) in the last section, and now see its behaviors against Δ. The numerical results are given in figure 4. From the figure, however, the witness W_3 cannot witness any QPT points. As we have seen, the negativity indeed signifies QPT points. There are three terms in the expression of negativity (26), and the competition among them leads to rich behaviors.

4. Conclusions

In the conclusion, we have given a general expression of negativity and an EW for the *XXZ* spin-1 model by considering several symmetries. In fact, it is applicable to more general models such as the following bilinear–biquadratic model with a single-ion anisotropy:

$$H = \sum_{i=1}^{N} \cos\theta (s_{ix}s_{i+1x} + s_{iy}s_{i+1y} + \Delta s_{iz}s_{i+1z}) + \sin\theta (s_{ix}s_{i+1x} + s_{iy}s_{i+1y} + \Delta s_{iz}s_{i+1z})^2 + D\sum_{i=1}^{N} s_{iz}^2. \qquad (28)$$

This simply because the three symmetries we used in the derivation of negativity in the *XXZ* model still exist in the above general model.

Using the analytical result of negativity, we have numerically investigated the negativity in the two spin-1 model, displaying QPTs. It was found that the negativity is an efficient indicator for QPT points. Although it cannot signify all, it indeed can identify many QPT points. Comparing two-site negativity and two-site entropy, the negativity is more sensitive to variation of parameters involved in the Hamiltonian, suggesting that it is a better indicator than the entropy. We also studied the behaviors of several EWs, and they can partly identify QPT points. Of course, one can use other EWs, which may work better than the present EWs. This deserves further investigations.

The method using negativity and EWs to study QPT is very convenient to use for numerical calculations, and it is applicable to higher-spin systems (not limited to spin-1 systems). One can also consider the case of more than two sites. But it is hard to get analytical results, and in addition, quantification of multipartite entanglement in higher-spin systems is very difficult. It is expected that the development of entanglement is very helpful to study QPT.

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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] Botet R and Jullien R 1983 *Phys. Rev.* B **27** 613
[6] Schollwöck, Jolicoeur T and Garel T 1996 *Phys. Rev.* B **53** 3304
[7] Betsuyaku H 1987 *Phys. Rev.* B **36** 799
[8] Sólyom J 1988 *Phys. Rev.* B **38** 11920
[9] Botet R, Jullien R and Kolb M 1983 *Phys. Rev.* B **28** 3914
[10] Osterloh A, Amico L, Falci G and Fazio R 2002 *Nature (London)* **416** 608
[11] Osborne T J and Nielsen M A 2002 *Phys. Rev.* A **66** 032110
[12] Fan H, Korepin V and Roychowdhury V 2004 *Phys. Rev. Lett.* **93** 227203
[13] Verstraete F, Martín-Delgado M A and Cirac J I 2004 *Phys. Rev. Lett.* **92** 087201
[14] Zhou L, Yi X X, Song H S and Quo Y Q 2003 *Preprint* quant-ph/0310169
[15] Gu S J, Tian G S and Lin H Q 2006 *New J. Phys.* **8** 61
[16] Legeza O and Sólyom J 2006 *Phys. Rev. Lett.* **96** 116401
[17] Peres A 1996 *Phys. Rev. Lett.* **77** 1413
Horodecki M, Horodecki P and Horodecki R 1996 *Phys. Lett.* A **223** 1
[18] Schliemann J 2003 *Phys. Rev.* A **68** 012309
Schliemann J 2005 *Phys. Rev.* A **72** 012307
[19] Breuer H P 2005 *Phys. Rev.* A **71** 062330
Breuer H P 2005 *J. Phys. A: Math. Gen.* **38** 9019
[20] Vidal G and Werner R F 2002 *Phys. Rev.* A **65** 032314
[21] Horodecki M, Horodecki P and Horodecki R 1996 *Phys. Lett.* A **223** 1
Terhal B M 2000 *Phys. Lett.* A **271** 319
Lewenstein M, Kraus B, Cirac J I and Horodecki P 2000 *Phys. Rev.* A **6** 052310
Lewenstein M, Kraus B, Cirac J I and Horodecki P 2001 *Phys. Rev.* A **63** 044304
[22] Wang X, Li H B, Sun Z and Li Y Q 2005 *J. Phys. A: Math. Gen.* **38** 8703
Zhang G M and Wang X 2006 *J. Phys. A: Math. Gen.* **39** 8515
[23] Tian G S and Lin H Q 2003 *Phys. Rev.* B **67** 245105
[24] Gu S J, Lin H Q and Li Y Q 2003 *Phys. Rev.* A **68** 042330