Entanglement properties in mixed spin-(1, s) systems

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Abstract

We obtain an exact expression of the negativity for SU(2)-invariant bipartite spin-(1, s) states via the partial time reversal method. Studies of thermal states show that the threshold temperature of entanglement may be arbitrary high when s is sufficient large, indicating that the entanglement is very robust against temperature. Negativities in bilinear-biquadratic system are also considered.

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1. Introduction

Entanglement has been considered as a fundamental resource of nature, which plays a key role in many interesting applications in quantum computation and quantum information [1–5]. For simplicity, people usually separate many-body systems into two parts when investigating entanglements. But how to measure the entanglement of high dimensional bipartite system is still an open question. Peres–Horodecki criterion [6–8] is very useful for high dimensional bipartite systems. Quantitatively, one can use the concept of negativity [9] to quantify entanglement. It is defined as \( \mathcal{N} = \sum_i |u_i| \), where \( u_i \) are negative eigenvalues of partial transposed (PT) density matrix \( \rho^{T_2} \), the operator \( T_2 \) denotes transposition respect to the second subsystem. Here, \( \rho \) is the density matrix of whole system. If \( \mathcal{N} > 0 \) the system is in an entangled state.

The symmetries of system could simplify the entanglement problem, and SU(2)-invariant states [10–15] have attracted much attention recently. Due to SU(2) symmetry, non-zero negativity is a necessary and sufficient condition for entanglement between a spin half and a spin \( s \) [10]. It has also been proved to be a necessary and sufficient condition for SU(2)-invariant entangled states [11,16,12] in bipartite Hilbert spaces with dimension \( 4 \times 4 \), and \( 3 \times M \) where \( M = 2j + 1 \) with \( j \) being an integer.

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In this paper we use partial time reversal (PTR) method [16] to investigate the spin systems. Time reversal is an antiunitary operator which commutes with all rotations and equivalent to the transposition operator up to local unitary operators [17]. A strong and computationally entanglement criterion has been constructed by using PTR method, it can detect the entangled positive partial transpose (PPT) state in one-parameter family of states [17]. The main idea of this paper is to replace the PT operation by time reversal operation which do not change the trace. We will see that PTR method is convenient to study negativities, it can reduce many calculations. We deduce an analytical formula for the negativity of spin-(1, s) SU(2)-invariant systems in Section 2 by using the PTR method. We can investigate entanglement properties exactly by negativity when s is an integer [12]. In Section 3, we use the analytical formula to investigate the entanglement of eigenstates and thermal states for a mixed spin-(1, s) system, we find that entanglement and quantum behavior can survive at arbitrary high temperature [18,19] when s is sufficient large.

Heisenberg models have been intensively used in the study of spin systems, recently research show that the interacting Hamiltonian may have higher powers of Heisenberg interactions when spin s is larger than $\frac{1}{2}$, those interacting systems display rich phase diagrams [20]. Among these Hamiltonians the bilinear-biquadratic [20–24] (BB) model plays an important role. In Section 4, we investigate the entanglement of spin-(1, s) BB model, we find that degenerate point of energies have close relation with negativities and may have some relation with quantum phase transition. For thermal states the temperature will smear those step-shaped negativities of ground state and excited states. The conclusions are given in Section 5.

2. An analytical result of negativity

Now, we first introduce the partial time reversal operation, and then give the analytical result of negativity for SU(2)-invariant state of mixed spin-(1, s) pair with s is an integer larger than 1.

It has been proved that time reversal operator acting on a operator $B$ can take the form of $V B^T V^\dagger$ [16,17], where $V$ is a unitary matrix representing a $\pi$-rotation about the y-axis. Joint operation, i.e., the partial transpose $\rho^{\tau_2}$ followed by a $\pi$-rotation along y-axis of the second spin $\exp(\pi i S_2^y)$ is the partial time reversal of density matrix with respect to the second system. We denote the PTR by $\tau_2$ in this paper. A unitary transformation will not influence the eigenvalues, so the negativity of PTR density matrix is the same as that of PT density matrix.

After some algebraic manipulations, the PTR of $s_1 \cdot S_2$ and its square term read

\[(s_1 \cdot S_2)^{\tau_2} = -s_1 \cdot S_2,\]

\[((s_1 \cdot S_2)^2)^{\tau_2} = (s_1 \cdot S_2)^2 + s_1 \cdot S_2.\]

The above equations are valid for any spin length $s_1$ and $s_2$, and are very useful for our derivation of the formula of the negativity.

Total spin $s_t$ of a bipartite spin system take values from $|s_1 - s_2|$ to $s_1 + s_2$, each one corresponds to an invariant subspace. Any SU(2)-invariant density matrix of the spin-(1, s) system can be written in the form of projectors

\[
\rho = \frac{x_{s+1}}{2s+3} P_{s+1} + \frac{x_s}{2s+1} P_s + \frac{x_{s-1}}{2s-1} P_{s-1},
\]

where the index of projector $P_{s_t}$ is the value of total spin $s_t$ and the coefficients $x_{s_t}$ can be expressed as a trace $\text{Tr}(\rho P_{s_t})$. Each $x_{s_t}$ is positive and summation of $x_{s_t}$ equals 1. Since

\[s_1 \cdot S_2 = \frac{1}{2}[(S_2 + s_1)^2 - S_2^2 - s_1^2] \sum_{s_t} P_{s_t},\]

\[= \sum_{s_t} \lambda_{s_t} P_{s_t},\]

we can also express its square term as line combination of projectors. For spin-(1, s) case it is

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\end{bmatrix}.
Conversely the projectors can be express as polynomial of \( s_1 \cdot S_2 \), the general form [26,25] of \( P_i \) for any spin length \( s_1 \) and \( s_2 \) is

\[
P_i = \prod_{s_i, s_\neq i} \frac{s_1 \cdot S_2 - \lambda_{s_i}}{\lambda_{s_i} - \lambda_i}.
\]

(6)

the property of \( P_i P_j = \delta_{ij} P_i \) has been used in the deduction. We write it explicitly For spin-(1, s) case in the following

\[
\begin{pmatrix}
P_{s+1} \\ P_s \\ P_{s-1}
\end{pmatrix}
= \begin{bmatrix}
\frac{1}{a} & \frac{s+2}{ab} & \frac{1}{ab} \\
1 & -\frac{s}{s+1} & \frac{1}{sa} \\
-\frac{1}{a} & -\frac{s}{s+1} & \frac{1}{sa}
\end{bmatrix}
\begin{bmatrix}
1 \\
\langle s_1 \cdot S_2 \rangle \\
\langle s_1 \cdot S_2 \rangle^2
\end{bmatrix},
\]

(7)

where \( a = 2s + 1, b = s + 1 \) and we name the coefficient matrix as \( M \). The \( x_{s_i} \) in Eq. (3) can then be achieved straightforwardly. Taking the expectation value of Eq. (7) we have

\[
\begin{pmatrix}
x_{s+1} \\ x_s \\ x_{s-1}
\end{pmatrix}
= [M]
\begin{bmatrix}
1 \\
\langle s_1 \cdot S_2 \rangle \\
\langle s_1 \cdot S_2 \rangle^2
\end{bmatrix},
\]

(8)

where \( \langle \rangle \) represents expectation value of any operator.

Instead of making partial transpose of the projectors we act \( \tau_2 \) on Eq. (7), make use of Eqs. (1) and (2), the PTR projectors read

\[
P_{s+1}^{\tau_2} = \frac{(s_1 \cdot S_2)^2}{(2s + 1)(s + 1)} - \frac{(s_1 \cdot S_2)}{(2s + 1)} + \frac{1}{2s + 1},
\]

\[
P_s^{\tau_2} = -\frac{(s_1 \cdot S_2)^2}{s(s + 1)} + 1,
\]

\[
P_{s-1}^{\tau_2} = \frac{(s_1 \cdot S_2)^2}{(2s + 1)s} + \frac{(s_1 \cdot S_2)}{(2s + 1)s} - \frac{1}{2s + 1}.
\]

(9)

Making Eq. (3) PTR we have

\[
\rho^{\tau_2} = C_1(s_1 \cdot S_2) + C_2(s_1 \cdot S_2)^2 + C_3,
\]

(10)

where \( C_1, C_2 \) and \( C_3 \) are constant, which are functions of \( s \) and \( x_{s_i} \) and can be easily calculated.

By virtue of Eq. (5), the PTR density matrix can be re-expressed as the summation of projectors and its eigenvalues can then be obtained easily.

\[
\rho^{\tau_2} = \frac{B_{s+1}}{2s + 3} P_{s+1} + \frac{B_s}{2s + 1} P_s + \frac{B_{s-1}}{2s - 1} P_{s-1},
\]

(11)

where

\[
B_{s+1} = \frac{1}{2s + 1} \left[ \frac{\langle(s_1 \cdot S_2)^2 \rangle}{s + 1} - (s_1 \cdot S_2) + 1 \right],
\]

\[
B_s = 1 - \frac{\langle(s_1 \cdot S_2)^2 \rangle}{s(s + 1)},
\]

\[
B_{s-1} = \frac{1}{2s + 1} \left[ \frac{\langle(s_1 \cdot S_2)^2 \rangle}{s} + (s_1 \cdot S_2) - 1 \right].
\]

(12)

The coefficients of \( P_{s_i} \) are the eigenvalues of PTR density matrix. They are the same as that of PT density matrix. Among them the one corresponding to the largest multiply subspace \( B_{s+1} \) is positive for it can be written as linear combination of \( x_{s_i} \) with positive coefficients.
Fig. 1. Negativities of eigenstates versus $s$ for different $s_t$.

The negativity $\mathcal{N}$ can be expressed as

$$\mathcal{N} = \max\{-B_{s-1}, 0\} + \max\{-B_s, 0\}$$

$$= \frac{1}{2s+1} \max\left\{1 - \langle s_1 \cdot S_2 \rangle - \frac{1}{s} \langle (s_1 \cdot S_2)^2 \rangle, 0\right\} + \frac{1}{s(s+1)} \max\{\langle (s_1 \cdot S_2)^2 \rangle - s(s+1), 0\}. \quad (13)$$

All those results are consistent with the work of Schliemann’s [10,11]. However, in their works, no expression of the negativity was given. We see that the two correlation functions are sufficient to determine the negativity, which greatly simplify the analysis of entanglement properties.

3. Apply results to a SU(2)-invariant bipartite system

We first apply the above results to eigenstates of SU(2) invariant system with Hamiltonian

$$H = s_1 \cdot S_2. \quad (14)$$

The two correlation functions can be obtained easily in this simple Hamiltonian. For spin-(1, $s$) case, $s_t = s - 1$ corresponds to the ground state (GS) with

$$\langle s_1 \cdot S_2 \rangle_g = -s - 1 \quad \langle (s_1 \cdot S_2)^2 \rangle_g = (s + 1)^2,$$

$$E_g = -s - 1 \quad \mathcal{N}_g = \frac{1}{s}. \quad (15)$$

The energy, spin correlators and negativity of the first excited state with $s_t = s$ are as follows

$$\langle s_1 \cdot S_2 \rangle_1 = -1 \quad \langle (s_1 \cdot S_2)^2 \rangle_1 = 1,$$

$$E_1 = -1 \quad \mathcal{N}_1 = \frac{2s - 1}{s(2s + 1)}. \quad (16)$$

We can see that the GS and the first excited state are entangled and their negativities are showed in Fig. 1 where the circle points represent negativity of GS and the star points represent that of the first excited state. The negativities are monotonously decreasing functions of $s$ and GS has relatively larger negativity than that of the first excited state until there are nearly no difference between them.

While for the second excited state $s_t = s + 1$ there is no entanglement at all since it has zero negativity and $s$ is integer. The energy and spin correlators of the second excited state read

$$\langle s_1 \cdot S_2 \rangle_2 = s \quad \langle (s_1 \cdot S_2)^2 \rangle_2 = s^2,$$

$$E_2 = s \quad \mathcal{N}_2 = 0. \quad (17)$$
Having known negativities of all eigenstates, we next consider thermal entanglement [22] of this system. Density matrix in thermal state is $\rho(T) = \exp(-\beta \hat{H})/Z$ where the partition function $Z = \text{Tr} \exp(-\beta \hat{H})$, $\beta = 1/k_BT$, $T$ is temperature, $k_B$ is Boltzmann’s constant and assumed to be 1. For spin-$\frac{1}{2}$ case, partition function reads

$$Z = (2s - 1)e^\beta(s+1) + (2s + 1)e^\beta + (2s + 3)e^{-\beta s}.$$  \hfill (18)

where the coefficients before exponential function are the number of degeneracy of the corresponding eigenstates.

We can obtain correlators $\langle (\vec{s}_1 \cdot \vec{s}_2)^n \rangle$ with $n$ being an arbitrary integer.

$$\langle (\vec{s}_1 \cdot \vec{s}_2)^n \rangle = \frac{(-1)^n}{Z} \frac{\partial^n}{\partial \beta^n} Z = [(2s - 1)(s + 1)^n e^{\beta(s+1)} + (2s + 1)e^\beta + (2s + 3)s^n(-1)^n e^{-\beta s}] \frac{(-1)^n}{Z}. \hfill (19)$$

In the following we write them explicitly up to the second order

$$\langle \vec{s}_1 \cdot \vec{s}_2 \rangle = -\frac{1}{Z}[(2s^2 + s - 1)e^{\beta(s+1)} + (2s + 1)e^\beta - (2s^2 + 3s)e^{-\beta s}],$$

$$\langle \vec{s}_1 \vec{s}_2 \rangle^2 = \frac{1}{Z}[(2s^3 + 3s^2 - 1)e^{\beta(s+1)} + (2s + 1)e^\beta + (2s^3 + 3s^2)e^{-\beta s}]. \hfill (20)$$

Substitute the above two equations into Eq. (12) we can obtain $B_{s-1}$, $B_s$ and $B_{s+1}$ where the $B_{s+1}$ and $B_{s-1}$ are always positive at any temperature (See Appendix). The negativity of thermal state is decided totally by $B_s$, it is

$$\mathcal{N}(T) = \max\{-B_s, 0\},$$

$$B_s = \frac{1}{s(s+1)Z} \{ e^{\beta(s+1)} (-2s^2 - s + 1) + e^\beta (2s + 1)(s^2 + s - 1) + e^{-\beta s} (2s^2 + 3s) \}. \hfill (21)$$

When $T \to 0$ the negativity reduces to $\frac{1}{2}$ for the GS, as we expected in Eq. (15).

In Fig. 2 we show the thermal negativities for several different $s$. For a given $s$, as temperature becomes higher the negativity becomes smaller, and there exists a threshold temperature $T_{th}$, after which negativity vanishes. We can see that as $s$ increases the $T_{th}$ become larger, it means entanglement is rather robust against temperature. When $S$ is infinite, one subsystem will behave classically and there is no negativity in the whole system. Numerical solving of equation $B_s = 0$ also shows that when $s$ is larger threshold temperature is higher. In the inset of Fig. 2 we show this property explicitly, for example $T_{th}(s = 1) \approx 1.37$, $T_{th}(s = 50) \approx 12.76$. Assume the system having meV as its energy unit, the corresponding threshold temperature of real physics is about 148 K for $s = 50$. Eq. (21) tells us that as $s$ approach infinity $T_{th}$ will be infinity, although the corresponding negativity becomes small. It means that entanglement can survive at high temperature. Compare the above results to that of spin-(1/2, $s$) system [19], we find those two systems have very similar properties, for the same $s$ the corresponding $T_{th}$ is higher in the spin-(1, $s$) system.
4. Bilinear-biquadratic model

In this section we consider the spin-(1, s) bilinear-biquadratic model with Hamiltonian

$$ H = \cos \theta s_1 \cdot S_2 + \sin \theta (s_1 \cdot S_2)^2. $$

(22)

For a given \( \theta \) there are three eigenstates belonging to different subspaces. For a fixed \( s \), i.e. in one subspace, energy will modulate with \( \theta \), and behave like sin function. The crossing points of energies of different subspaces satisfy one of the following equations

$$ E_{s+1} = E_{s-1} = -\frac{s}{\sqrt{2}} - \frac{s^2}{\sqrt{2}} \tan \theta = 1, $$

$$ E_s = E_{s-1} = \frac{-s}{\sqrt{1 + (s-1)^2}} \tan \theta = \frac{1}{s + 2}, $$

$$ E_s = E_{s+1} = \frac{-s - 1}{\sqrt{1 + (s+2)^2}} \tan \theta = \frac{1}{1 - s}, $$

(23)

where the indexes of \( E \) denote the value of \( s \), and here we give the expression of energy. In Fig. 3(a) we take \( s = 2 \) as an example to show how do the energies of eigenstates with fixed \( s \) modulate as \( \theta \) go through its period, \( \theta_i, \ i = 1, 2, 3 \) denote the three degenerate points of ground state with excited states. The other three crossing points have \( \pi \) distance away from them. For a finite \( s \), the GS will change three times from one subspace to another subspace, and the behavior of negativity is shown in Fig. 3(b). At those energy degenerate point, negativity will change from a steady value to another one.

For the first and second excited states, in no-limiting case there are six and three energy degenerate points respectively, the negativities also jump from a steady value to another one which we show in Fig. 4(a) and (b). It gives a hint that energy degeneration, entanglement may have close relation with quantum phase transition [27] as many people advocate.

Now, we take a look of the energy degenerate points which may correspond to the points of quantum phase transitions. We can see from Figs. 3(b) and 4 that there exist degenerate points which are independent of \( s \) with arctan \( \theta = 1 \), the \( \pi/4 \) and \(-3\pi/4\) point are the bound [20,28] of phase transition in BB spin-1 chain system. From the Eq. (23) we find that as \( s \) increase from 1 to \( \infty \), \( \theta_2 \) decrease from arctan(1/4) to 0, while \( \theta_3 \) increase from \( \frac{\pi}{2} \) to \( \pi \). We plot how does the corresponding degenerate points modulate in Fig. 5 for \( s = 1 \ldots 10 \), it shows that as \( s \) increase the segment of I will be full-filled which happen to be a part of the ferromagnetic phase of BB spin-1 chain [20,28].
Fig. 4. (a) The negativity of the first excited state vs $\theta$ for different $s$. (b) The negativity of the second excited state vs $\theta$ for different $s$.

Fig. 5. As $s$ increase from 1, the degenerate point modulate along the arrow directs.

Fig. 6. The negativities of the thermal states of BB model for a given $s$ with different temperature, where (a) for $s = 2$ case and (b) for $s = 4$ case.

As temperature increase from zero, we plot the corresponding negativities of thermal state which we show in Fig. 6. We can see that the steady value of negativity will be destroyed by temperature. We can also see that for larger $s$ it will need higher temperature to smear the perfect steady value of eigenstates.
5. Conclusion

In conclusion, we obtain the negativity analytically by using PTR method for bipartite SU(2)-invariant spin-(1, s) system. One merit of our PTR approach is that it can be applicable for spin-(1, s) systems with arbitrary s. For each s, negativity can be expressed as function of its correlators. Applying our results to the Heisenberg spin system, we find that the ground state and the first excited state are entangled, the entanglement decrease with increased s. While for integer s the second excited state is separate. Concerning about thermal state, its correlators can be expressed as derivative of its partition function. Entanglement will decreases with increasing temperature, and the \( T_{th} \) which correspond to zero negativities become higher with larger s. Entanglement can exist in very high temperature.

We also consider a SU(2)-invariant spin-1 spin-s BB model. When the GS and excited states turn from one subspace to another subspace, their negativities change from a steady value to another steady value. As s increase we studied the degenerate points vs s. Temperature will smear the steady value of negativities. We show that the negativity jump points exactly reflect the energy degenerate points, which may possibly correspond to quantum phase transition.

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Appendix

In the thermal state we have:

\[
B_{s+1} = \frac{1}{z} \frac{1}{2s + 1} \frac{1}{s + 1} \{e^{-\beta_s}(2s + 3) + e^{\beta}(4s^2 + 8s + 3) + e^{\beta(s+1)}(4s^3 + 8s^2 + s - 3)\},
\]

it straightforward to see that \( B_{s+1} \) is always larger than zero since \( s \geq 1 \). About \( B_{s-1} \) it can be written as:

\[
B_{s-1} = \{-e^{\beta(s+1)}(2s + 1) + s(2s + 3) + e^{\beta(2s+1)}\} \times \frac{1}{z} \frac{1}{2s + 1} \frac{1}{s} (2s - 1)e^{-\beta_s}.
\]

(24)

In the above equation if what inside the \{\} larger than zero then \( B_{s-1} > 0 \). The minimal point of \{\} can obtain by doing derivation of \( \beta \) which satisfied

\[
e^{\beta_s(2s+1)} = (s + 1)e^{\beta_s(s+1)},
\]

\[
\beta_s = \frac{\ln(s + 1)}{s}.
\]

(25)

Substitute the above equation into \{\} of Eq. (24) we find the minimal point of \{\} equals \( s[2s + 3 - (s + 1)^{1+1/s}] \). We can use induction method to prove \( 2 > (1 + s)^{1/s} \) and then

\[
2 > (1 + s)^{1/s} - \frac{1}{s + 1}, \quad \frac{2s + 3}{s + 1} > (1 + s)^{1/s}.
\]

(26)

It means the minimal point of \{\} is larger than zero so that the function \( B_{s-1} \) is always larger than zero.

References