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Genuine tripartite entanglement and quantum phase transition*

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A new simplified formula is presented to characterize genuine tripartite entanglement of $(2 \otimes 2 \otimes n)$-dimensional quantum pure states. The formula turns out equivalent to that given in (*Quant. Inf. Comp.* **7**(7) 584 (2007)), hence it also shows that the genuine tripartite entanglement can be described only on the basis of the local $(2 \otimes 2)$-dimensional reduced density matrix. In particular, the two exactly solvable models of spin system studied by Yang (*Phys. Rev.* A **71** 030302(R) (2005)) are reconsidered by employing the formula. The results show that a discontinuity in the first derivative of the formula or in the formula itself of the ground state just corresponds to the existence of quantum phase transition, which is obviously different from the concurrence.

Keywords: entanglement measure, tripartite entanglement, quantum phase transition
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1. Introduction

Quantum entanglement is one of the most fascinating features of quantum mechanics and is a crucial physical resource in much quantum information processing. It has attracted much attention in recent years. Even though a great deal of effort has been made to characterize quantitatively the entanglement properties of a quantum system,[1−12] however, good understanding is still restricted to low-dimensional systems. The quantification of entanglement for higher-dimensional systems and multipartite quantum systems remains an open question.

It has been shown that there are some good reasons to study entanglement in multipartite quantum systems.[13−16] In particular, quantum entanglement in the ground state of strongly correlated systems has attracted many physicists' interest.[17−28] Most of the works focused on the spin models. They employed the remarkable bipartite entanglement measure-concurrence[1] to measure the entanglement of a pair of nearest-neighbour particles (in this paper, 'concurrence' always refers to the concurrence of a pair of nearest-neighbour particles for simplification, if there are not other statements), and attempted to understand the connection between quantum entanglement (QE) and quantum phase transitions (QPT). Even though it has been found in some works (for example, Refs.[22,25]) that the critical behaviours of the concurrence such as a discontinuity in concurrence or its first derivative of the ground state can signal a QPT (first-order QPT (1QPT) or second-order QPT (2QPT) may be included), they are usually not universal. A lot of examples[17,19−21,29] have shown that the critical behaviours of concurrence of the ground state cannot faithfully reflect the QPT of the given models. In particular, in Ref.[21], the author found that the discontinuity of the first derivative of concurrence for the exactly solvable quantum spin-$\frac{1}{2}$ XY model with three-spin interactions[30] does not signal any quantum critical points. They also showed that the discontinuity of the first derivative of concurrence for the XXZ spin chain corresponds to a 1QPT instead of 2QPT. Hence, concurrence may not be a good candidate to connect QE with QPT, even though concurrence indeed does well in some models. In fact, QPT should be an embodiment of some collective behaviours of a multipartite systems, while concurrence only describes some relation (entanglement or separability) between a pair of local particles. It is an inevitable shortcoming for concurrence to capture some collective behaviours.[13]

In this paper, we present a simplified formula to characterize the entanglement of tripartite $(2\otimes2\otimes n)$-dimensional quantum pure states. It has been proved

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to be an equivalent expression to that in Ref.[31]. That is to say, not only can the formula here characterize the properties of genuine tripartite entanglement, but also it can be considered as a 'good' entanglement measure if one does not consider local operations in the higher-dimensional subsystem (local unitary transformations excluded). However, the distinct advantage of the current formula is that it can significantly simplify that formula in Ref.[31]. To measure the genuine tripartite entanglement, it is not necessary to obtain the total density matrix of the $(2\otimes 2\otimes n)$-dimensional quantum pure states, but only the local $(2\otimes 2)$-dimensional reduced density matrix. As an example, we reconsider the two models of spin system presented in Ref.[21] and employ our measure to calculate the genuine tripartite entanglement by considering the whole spin chain as a $(2\otimes 2\otimes n)$-dimensional quantum pure state. The results indicate that our measure can faithfully signal the 2QPT point of the spin-$\frac{1}{2}$ XY model and the 1QPT point at $\Delta=-1$ of the XXZ model. The paper is organized as follows. We first introduce the new formula for genuine tripartite entanglement and then apply the measure to the two spin models. The conclusion is drawn at the end.

2. The new formula of genuine tripartite entanglement measure

Consider a tripartite $(2\otimes 2\otimes n)$-dimensional pure state given in computational basis by

$$|\psi_{ABC}\rangle=\sum_{i,j=0}^{1}\sum_{k=0}^{n-1}a_{ijk}\,|i\rangle_A\,|j\rangle_B\,|k\rangle_C\,, \tag{1}$$

with $\sum\limits_{i,j=0}^{1}\sum\limits_{k=0}^{n-1}|a_{ijk}|^2=1$, and the reduced density matrix by tracing over party C is denoted by ρ_{AB}, a $(2\otimes 2)$-dimensional matrix. Based on the Pauli matrix $\sigma_y=\begin{pmatrix}0&-i\\ i&0\end{pmatrix}$, the spin-flipped state denoted by $\tilde{\rho}_{AB}$ can be obtained by

$$\tilde{\rho}_{AB}=(\sigma_y\otimes\sigma_y)\,\rho_{AB}^{*}\,(\sigma_y\otimes\sigma_y)\,, \tag{2}$$

where ρ_{AB}^{*} stands for the complex conjugate of ρ_{AB}.

Theorem 1 The $\tau(|\psi_{ABC}\rangle)$ that characterizes the genuine tripartite entanglement of $|\psi_{ABC}\rangle$ defined in $(2\otimes 2\otimes n)$-dimensional Hilbert space can be given by

$$\begin{aligned}&\tau(|\psi_{ABC}\rangle)\\ &=\sqrt[4]{\left[\mathrm{tr}\left(\rho_{AB}\tilde{\rho}_{AB}\right)\right]^2-\mathrm{tr}\left[\left(\rho_{AB}\tilde{\rho}_{AB}\right)^2\right]},\end{aligned} \tag{3}$$

where $\mathrm{tr}(\cdot)$ denotes the trace operation of a matrix.

Proof For a pure state $|\psi_{ABC}\rangle$, the corresponding reduced density matrix ρ_{AB} can usually be expressed as a bipartite mixed state as

$$\rho_{AB}=\sum_i p_i\,|\varphi_i\rangle\,\langle\varphi_i|\,,\sum_i p_i=1, \tag{4}$$

according to any decomposition of ρ_{AB} (Note that ρ_{AB} may be a pure state, which can be considered as a special case of Eq.(4) with $p_1=1$ and $p_{i\neq 1}=0$). The matrix notation of Eq.(4) can be given by $\rho_{AB}=\Psi W\Psi^{\dagger}$, where the columns of Ψ corresponds to $|\varphi_i\rangle$ and W is a diagonal matrix with its diagonal entries corresponding to p_i respectively. Therefore, Eq.(3) can be rewritten by

$$\begin{aligned}&\tau^4(|\psi_{ABC}\rangle)\\ &=\left\{\mathrm{tr}\left[\Psi W\Psi^{\dagger}\,(\sigma_y\otimes\sigma_y)\,\Psi^{*}W\Psi^{\mathrm{T}}\,(\sigma_y\otimes\sigma_y)\right]\right\}^2\\ &\quad-\mathrm{tr}\left[\Psi W\Psi^{\dagger}\,(\sigma_y\otimes\sigma_y)\,\Psi^{*}W\Psi^{\mathrm{T}}\,(\sigma_y\otimes\sigma_y)\right]^2,\end{aligned} \tag{5}$$

with the superscript T denoting transpose operation. By a small change of Eq.(5), one can obtain

$$\begin{aligned}&\tau^4(|\psi_{ABC}\rangle)\\ &=\{\mathrm{tr}[\sqrt{W}\,\Psi^{\dagger}\,(\sigma_y\otimes\sigma_y)\,\Psi^{*}\sqrt{W}\\ &\quad\cdot\sqrt{W}\,\Psi^{\mathrm{T}}\,(\sigma_y\otimes\sigma_y)\,\Psi\sqrt{W}]\}^2\\ &\quad-\mathrm{tr}[\sqrt{W}\,\Psi^{\dagger}\,(\sigma_y\otimes\sigma_y)\,\Psi^{*}\sqrt{W}\\ &\quad\cdot\sqrt{W}\,\Psi^{\mathrm{T}}\,(\sigma_y\otimes\sigma_y)\,\Psi\sqrt{W}]^2,\end{aligned} \tag{6}$$

where $\sqrt{W}$ stands for the square root of the entries of W.

Recalling the procedure of constructing the genuine tripartite entanglement in Ref.[31], one has to project $|\psi_{ABC}\rangle$ onto the subspace of Party C and obtain a set of unnormalized bipartite pure states. If assuming that every element of the set just corresponds to $\sqrt{p_i}\,|\varphi_i\rangle$ given by Eq.(4), in other words, $\Psi\sqrt{W}$ is just the matrix notation of $\{\sqrt{p_i}\,|\varphi_i\rangle\}$, one can easily find that

$$\begin{aligned}&\tau^4(|\psi_{ABC}\rangle)\\ &=\left[\mathrm{tr}\left(\mathcal{M}\mathcal{M}^{\dagger}\right)\right]^2-\mathrm{tr}\left[\left(\mathcal{M}\mathcal{M}^{\dagger}\right)^2\right],\end{aligned} \tag{7}$$

where $\mathcal{M}=\sqrt{W}\,\Psi^{\mathrm{T}}\,(\sigma_y\otimes\sigma_y)\,\Psi\sqrt{W}$. Equation (7) is consistent with that in Ref.[31]. Therefore, $\tau(|\psi_{ABC}\rangle)$

is an entanglement semi-monotone of genuine tripartite entanglement.

The distinct advantage of current version given in Eq.(3) is that $\tau(|\psi_{ABC}\rangle)$ can be easily obtained from the reduced density matrix instead of obtaining the total pure state $|\psi_{ABC}\rangle$ by following the complicated procedure given in Ref.[31]. In fact, Eq.(3) is also a simplification of the genuine tripartite entanglement measure of $(2\otimes 2\otimes 2)$-dimensional pure states given in Ref.[5]. The advantage is something like the case of bipartite entanglement measure, i.e. the linear entropy (or its analogue[12]) of a bipartite entangled pure state can be considered as an analogous simplification[1] of the length of concurrence vector.[3] One will find that the simplification makes the application of our measure more convenient. Furthermore, for the extension of Eq.(3) to mixed states, one will have to turn to the procedure given in Ref.[31].

3. The signal of quantum phase transition

Now, let us reconsider the isotropic spin-$\frac{1}{2}$ XY chain with three-spin interaction presented in Refs.[18,27], which is an exactly solvable quantum spin model. The Hamiltonian is

$$H = -\sum_{i=1}^{N}\Big[\sigma_i^x\sigma_{i+1}^x+\sigma_i^y\sigma_{i+1}^y + \frac{\lambda}{2}\left(\sigma_{i-1}^x\sigma_i^z\sigma_{i+1}^y-\sigma_{i-1}^y\sigma_i^z\sigma_{i+1}^x\right)\Big], \qquad (8)$$

where N is the number of sites, $\sigma_i^\alpha(\alpha=x,y,z)$ are the Pauli matrices, and λ is a dimensionless parameter characterizing the three-spin interaction strength. Here the periodic boundary condition $\sigma_{N+1}=\sigma_1$ is assumed. Reference [27] has shown that the three-spin interaction can lead to a 2QPT at $\lambda=\lambda_C=1$. However, Ref.[18] has shown that the discontinuity of the first derivative of the ground-state concurrence of the nearest–neighbour spins cannot dependably signal a QPT, because there does not exist any QPT at $\lambda=2/(\sqrt{2}-1)\pi$, but the first derivative of the ground-state concurrence shows discontinuity here. Furthermore, Ref.[18] has shown that the von Neumann entropy[23] as an entanglement measure, defined as $S=-\mathrm{tr}(\rho_j\log_2\rho_j)$, also fails to detect the QPT of the current model, where ρ_j is the one-particle reduced density matrix. It is natural to wonder whether the entanglement measure given by Eq.(3) can well detect the QPT of the model.

Since the total ground state can be considered as a tripartite $(2\otimes 2\otimes n)$-dimensional pure state, and in particular, it is not necessary to introduce local operations to such as Positive Operator Values Measure and so on for a given spin system, the entanglement measure presented previously can be safely employed to measure the entanglement by which we will investigate the QPT in the model. Due to the entanglement measure given by Eq.(3), it is necessary to only obtain the two-nearest-neighbour-particle reduced density matrix which has been in fact given in Ref.[21]. On the basis of the Hamiltonian given in Ref.[21], the two-nearest-neighbour-particle reduced density matrix by tracing over other spins can be given by[24]

$$\rho_{i,i+1}=\begin{pmatrix} u_{i,i+1} & 0 & 0 & 0\\ 0 & w_{i,i+1} & z_{i,i+1} & 0\\ 0 & z_{i,i+1} & w_{i,i+1} & 0\\ 0 & 0 & 0 & u_{i,i+1}\end{pmatrix} \qquad (9)$$

in the standard basis $\{|\uparrow\uparrow\rangle,|\uparrow\downarrow\rangle,|\downarrow\uparrow\rangle,|\downarrow\downarrow\rangle\}$, where

$$u_{i,i+1}=\frac{1}{4}(1-G^2),$$

$$w_{i,i+1}=\frac{1}{4}(1+G^2),$$

and

$$z_{i,i+1}=G/2, \qquad (10)$$

with

$$G=\begin{cases}\dfrac{2}{\pi}, & \lambda<1,\\ \dfrac{2}{\pi\lambda}, & \lambda\geq 1.\end{cases} \qquad (11)$$

Hence, the entanglement measure τ_{XY} can be easily obtained in terms of Eq.(3), which is given in Fig.1. Figure 1 shows that τ_{XY} is continuous for all λ and the first derivative of τ_{XY} is only discontinuous at $\lambda=\lambda_C=1$, which indicates the 2QPT only at λ_C.

Another model considered in Ref.[21] is the one-dimensional XXZ model,

$$H_{XXZ}=\sum_{i=1}^{N}\left[\sigma_i^x\sigma_{i+1}^x+\sigma_i^y\sigma_{i+1}^y+\Delta\sigma_i^z\sigma_{i+1}^z\right]. \qquad (12)$$

The model has shown that there exist a 1QPT instead of 2QPT at the critical point $\Delta=-1$. However, the concurrence of the nearest-neighbour-two-particle reduced density matrix is continuous at $\Delta=-1$, while the first derivative of the concurrence is not continuous at the critical point. This behaviour of concurrence associated with its derivative shows a 2QPT of

the model, which is, in this sense, opposite to the fact concluded in Ref.[21] that the nonanalyticity would mislead in detection of a QPT. However, one will find that the nonanalyticity of our measure τ can just show a 1QPT of the model at $\Delta = -1$.

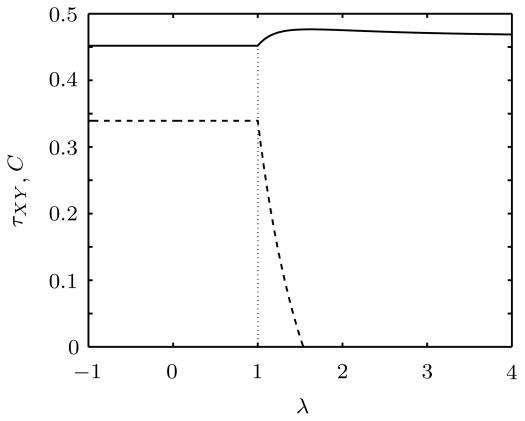


Fig.1. The genuine tripartite entanglement τ_{XY} (solid line) and the concurrence C (dashed line) of the ground state of the isotropic spin-$\frac{1}{2}$ XY chain versus the three-spin interaction strength λ. The figure (Dimensionless) shows obviously that $\frac{\partial \tau_{XY}}{\partial \lambda}$ is discontinuous at $\lambda = 1$, which signals only one 2QPT.

Based on Refs.[21,24], the nearest-neighbour-two-particle reduced density matrix has the same form as Eq.(9). The elements can be obtained from Ref.[21] as

$$u_{i,i+1} = \frac{1}{4}\left(1 + \frac{\partial \mathcal{E}}{\partial \Delta}\right), \tag{13}$$

$$z_{i,i+1} = \frac{1}{4}\left(\mathcal{E} - \Delta \frac{\partial \mathcal{E}}{\partial \Delta}\right), \tag{14}$$

where $\mathcal{E} = \langle \sigma_i^x \sigma_{i+1}^x \rangle + \langle \sigma_i^y \sigma_{i+1}^y \rangle + \Delta \langle \sigma_i^z \sigma_{i+1}^z \rangle$ is the ground-state energy per site in the XXZ model. At $\Delta = -1$, one has $\mathcal{E}|_{\Delta=-1} = -1$.[21,32] Substituting Eq.(9) associated with Eqs.(13,14) into Eq.(3), one will obtain the corresponding genuine tripartite entanglement measure τ_{XXZ}, which can be formally written by

$$\tau_{XXZ} = f\left(\frac{\partial \mathcal{E}}{\partial \Delta}\right), \tag{15}$$

where $f(x)$ is a continuous function on x, which can be found by Eq.(3). From Refs.[21,32], one can also find that $\left.\frac{\partial \mathcal{E}}{\partial \Delta}\right|_{\Delta \to -1^+} \to 0$ and $\left.\frac{\partial \mathcal{E}}{\partial \Delta}\right|_{\Delta < -1} = 1$. That is to say, $\frac{\partial \mathcal{E}}{\partial \Delta}$ is not continuous at $\Delta = -1$. Thus one can conclude that τ_{XXZ} is not continuous at $\Delta = -1$ due to the property of $f(x)$. This result indicates that the discontinuity of τ_{XXZ} at $\Delta = -1$ signals a 1QPT. However, the other critical point of the model at $\Delta = 1$ does not correspond to the discontinuous behaviour of τ_{XXZ} or its first derivative, which is analogous to the concurrence. In fact, numerical results based on Refs.[33,34] can show that τ_{XXZ} reaches its minimum at $\Delta = 1$. The result is not given here.

4. Conclusion and discussions

We have presented a simplified formula to characterize genuine tripartite entanglement of $(2 \otimes 2 \otimes n)$-dimensional quantum pure states. It has been proved that the formula is an equivalent description of the genuine tripartite entanglement introduced in Ref.[31]. The distinct advantage is that the current formula can be obtained only by using the local $(2 \otimes 2)$-dimensional reduced density matrix, which significantly simplifies the calculation of the genuine tripartite entanglement introduced in Ref.[31] including the original one in Ref.[5]. This is something like the case of bipartite entanglement measure, i.e. the linear entropy as a simplification of the length of concurrence vector can be obtained by the reduced matrix. By employing the new measure, we reconsider the two exactly solvable spin models presented in Ref.[21]. The results have shown that a discontinuity in the first derivative of the entanglement measure or in the entanglement measure itself of the ground state just corresponds to the existence of quantum phase transitions. Of course, the measure cannot always work well, for example, at the critical point $\Delta = 1$ for XXZ model, neither τ_{XXZ} nor $\frac{\partial \tau_{XXZ}}{\partial \Delta}$ shows discontinuous behaviour. From the block–block–block entanglement point of view, it is implied that the spin chain is considered as tripartite quantum states, including two 2-dimensional blocks. The other treatments such as three higher-dimensional blocks, even multiple higher-dimensional blocks, may be more effective for the detection of QPT. In this sense, the generalization of τ to higher-dimensional systems and multipartite systems seems to be needed.

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