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Sufficient and necessary conditions of separability for bipartite pure states in infinite-dimensional systems

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The PHC criterion and the realignment criterion for pure states in infinite-dimensional bipartite quantum systems are given. Furthermore, several equivalent conditions for pure states to be separable are generalized to infinite-dimensional systems.

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In quantum mechanics, the states of the system are described by density operators which are positive linear operators on a complex Hilbert H with unit trace and the observables are represented by self-adjoint operators on H. A density operator that is a projection on a single vector is referred to as representing a pure state, while other density operators are representing mixed states.

Let H and K be complex separable Hilbert spaces and the tensor product Hilbert space $H\otimes K$ be the corresponding bipartite quantum system. By $S(H)$, $S(K)$ and $S=S(H\otimes K)$, we denote the sets of states on H, K and $H\otimes K$, respectively. Recalling that, a pure state $\rho\in S$ is called separable if, as the same to the finite-dimensional systems, $\rho=\rho^{(1)}\otimes\rho^{(2)}$, a mixed state $\rho\in S$ is called separable if it can be written as a convex combination

$$\rho=\sum_i p_i\rho_i^{(1)}\otimes\rho_i^{(2)}, \qquad (1)$$

or can be approximated in the trace norm by the states of the above form [1,2], where the series converges in trace norm, $\rho^{(1)}$, $\rho_i^{(1)}$ and $\rho^{(2)}$, $\rho_i^{(2)}$ are pure states in $S(H)$ and $S(K)$, respectively; $\sum_i p_i=1$, $p_i\geqslant 0$. Or else, ρ is called entangled (or inseparable). We denote by S_0 the set of all separable states in S.

The quantum entangled states have been used as a basic resource in quantum information processing and communication [3,4], such as quantum cryptography [5,6], quantum computation [7,8], quantum secret sharing [9,10], quantum dense coding [11] and so on. Recently, entanglement in different models are investigated, for instance, the Jaynes-Cummings model [12], the Heisenberg XXZ model [13,14], the QED model [15] and the CV photon model [16]. To decide whether or not a state of bipartite quantum system is entangled is one of the most challenging tasks of this field [3,17]. For the finite-dimensional case, several entanglement criteria are proposed, such as the "positive partial transposition (PPT) criterion" [18,19], the "partial Hermitian conjugate (PHC) criterion" (a criterion for pure states [20]) and the 'realignment criterion' [21–24]. It is known that a pure state $\rho=|\psi\rangle\langle\psi|$ in a finite-dimensional system is separable if and only if one of the following statements is true: (i) ρ is PPT; (ii) ρ is invariant under PHC; (iii) the trace norm of the realignment matrix of ρ is 1. It is interest-

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ing to ask whether or not these criteria are still true for the pure states in infinite-dimensional systems. In this note, we generalize the PHC criterion and the realignment criterion to infinite-dimensional case and give some sufficient and necessary conditions for bipartite pure states in infinite-dimensional systems to be separable. We show that, for a pure state $\rho=|\psi\rangle\langle\psi|\in S(H\otimes K)$ with dim$H=\infty$ or dim$K=\infty$, the following conditions are equivalent: (1) ρ is separable; (2) ρ is PPT; (3) ρ is invariant under PHC; (4) $\|D_\psi\|=1$; (5) $\|\rho^R\|_{\mathrm{Tr}}=1$, where D_ψ is the coefficient operator of $|\psi\rangle$ (defined in the next paragraph), ρ^R denotes the realignment operator of ρ and $\|\cdot\|_{\mathrm{Tr}}$ stands for the trace norm.

Throughout this note, $\{|i\rangle\}$ and $\{|j\rangle\}$ stand for the orthonormal bases of H and K, respectively. For a vector $|\psi\rangle=\sum_{i,j}d_{ij}|i\rangle|j\rangle\in H\otimes K$, denote by $D_\psi=(d_{ij})$ the coefficient operator of $|\psi\rangle$, which may be regard as an operator from K into H defined by $D_\psi(|j\rangle)=\sum_i d_{ij}|i\rangle$. Clearly, D_ψ is a Hilbert-Schmidt operator with the Hilbert-Schmidt norm $\|D_\psi\|_2=\||\psi\rangle\|$. Thus D_ψ is bounded and we denote its operator norm by $\|D_\psi\|$, that is, $\|D_\psi\|=\sup_{\||x\rangle\|\le 1}\|D_\psi|x\rangle\|$. For a density operator ρ, we denote by ρ^{T_1}, ρ^{T_2} the partial transpositions of ρ with respect to the first and second subsystems, respectively.

1 Partial Hermitian conjugate criterion for pure states

In this section, we introduce the concept of partial Hermitian conjugate (PHC) of pure states in infinite-dimensional bipartite systems, and generalize the PHC criterion in [20] to infinite-dimensional case.

At first, we give the definition of PHC for separable pure states. For a separable pure state $\rho=|\psi\rangle\langle\psi|$ with $|\psi\rangle=\sum_{i,j}d_{ij}|i,j\rangle$, we can write $d_{ij}=a_ib_j$, where a_i and b_j are the coefficients with respect to $|i\rangle$ and $|j\rangle$, respectively. That is

$$|\psi\rangle=\sum_{i,j}a_ib_j|i,j\rangle$$

and therefore the density operator is

$$\rho=|\psi\rangle\langle\psi|=\sum_{i,j,i',j'}a_ib_j\overline{a_{i'}b_{j'}}\,|i,j\rangle\langle i',j'|.$$

Then, similar to the finite-dimensional case, the partial Hermitian conjugate of ρ is defined by

$$\rho^{\mathrm{PHC}}=|\psi\rangle\langle\psi|=\sum_{i,j,i',j'}a_i\overline{b_j}\,\overline{a_{i'}}b_{j'}\,|i,j'\rangle\langle i',j|.$$

However, for a general bipartite pure state, it is uneasy to calculate its partial Hermitian conjugate since it also needs complex conjugation on the corresponding coefficients [20]. To avoid this difficulty, we consider the so-called Schmidt decomposition of a given unit vector in $H\otimes K$. Notice that, similar to the finite-dimensional case, each vector in infinite-dimensional tensor product Hilbert space of two Hilbert spaces has a Schmidt decomposition [25]. In [25], Blanchard et al. proposed a proof for the Schmidt decomposition for a vector in $H\otimes K$. In what follows, we give another simple proof.

Lemma 1.1 (**Schmidt's decomposition [25]).** Let H and K be complex Hilbert spaces, and let $|\psi\rangle\in H\otimes K$ be a unit vector. Then there exist orthonormal sets $\{|k\rangle\}$ and $\{|k'\rangle\}$ of H and K, respectively, and positive numbers λ_1, λ_2, $\cdots$ with $\sum_k\lambda_k^2=1$, such that

$$|\psi\rangle=\sum_k\lambda_k|k,k'\rangle.$$

Proof. Taking any orthonormal bases $\{|i\rangle\}$ and $\{|j\rangle\}$ of H and K, respectively. Then there exist scalars d_{ij}, with at most countable many nonzero, such that $|\psi\rangle=\sum_{i,j}d_{ij}|i,j\rangle$. Let $D=D_\psi=(d_{ij})$. D is a Hilbert-Schmidt operator. Consider the polar decomposition $D=W|D|$ of D, where $|D|=(D^\dagger D)^{\frac{1}{2}}$ and W is a partial isometry on $H\otimes K$. As $|D|$ is compact, by the spectrum theorem, there exists a sequence $\{P_k\}$ of rank-one projections with $P_kP_{k'}=0$ if $k\neq k'$, and a sequence of positive numbers $\{\lambda_k\}$ with $\lambda_k\geqslant\lambda_{k'}$ if $k<k'$, such that $|D|=\sum_k\lambda_kP_k$. It is clear that there exists a unitary operator $V=(v_{ij})$ such that $|D|=VSV^\dagger$ with $S=\mathrm{diag}(\lambda_1,\lambda_2,\cdots)$. Let $U=WV^\dagger$. It follows that

$$D=W|D|=WVSV^\dagger=USV^\dagger. \tag{2}$$

Thus

$$|\psi\rangle=\sum_{i,j}d_{ij}|i,j\rangle=\sum_{i,j,k}u_{ik}\lambda_kv_{kj}|i,j\rangle.$$

Define $|k\rangle=\sum_i u_{ik}|i\rangle$ and $|k'\rangle=\sum_j v_{kj}|j\rangle$, we arrive at

$$|\psi\rangle=\sum_{i,j,k}u_{ik}\lambda_kv_{kj}|i,j\rangle=\sum_k\lambda_k|k,k'\rangle.$$

Note that $|k\rangle$ and $|k'\rangle$ are orthonormal sets since U and V are unitary operators.

It is clear that $\sum_i \lambda_k^2 = 1$ since $|\psi\rangle$ is a unit vector. ■

As one might expect, if $|\psi\rangle = \sum_k \lambda_k |k,k'\rangle$ is the Schmidt decomposition of $|\psi\rangle$, then the Schmidt coefficients of $|\psi\rangle$, $\{\lambda_k\}$ are uniquely determined by $|\psi\rangle$ since $\{\lambda_k\}$ are the nonzero eigenvalues of the reduced Hilbert-Schmidt operator. We call the orthonormal bases of H and K extended by $\{|k\rangle\}$ and $\{|k'\rangle\}$ the Schmidt bases of $|\psi\rangle$.

By the lemma above, we give the following definition.

Definition 1.2. Let $\rho = |\psi\rangle\langle\psi|$ be a pure state in $S(H\otimes K)$ and $|\psi\rangle = \sum_k \lambda_k |k,k'\rangle$ be the Schmidt decomposition of $|\psi\rangle$. Then

$$\rho = \sum_{k,l} \lambda_k \lambda_l |k,k'\rangle\langle l,l'|$$

and the partial Hermitian conjugate of ρ is defined by

$$\rho^{\text{PHC}} = \sum_{k,l} \lambda_k \lambda_l |k,l'\rangle\langle l,k'|.$$

Remark that, for any given pure state $\rho = |\psi\rangle\langle\psi|$, as the Schmidt decomposition of $|\psi\rangle$ is uniquely determined, ρ^{PHC} is uniquely determined and thus the PHC operation for pure states is well defined.

We are now ready to prove the PHC criterion for the infinite-dimensional case.

Criterion 1.3 (**PHC criterion**). Let $\rho = |\psi\rangle\langle\psi| \in S(H\otimes K)$ be a pure state, then ρ is separable if and only if $\rho^{\text{PHC}}=\rho$.

Proof. If $\rho = |\psi\rangle\langle\psi|$ is a separable pure state and $|\psi\rangle = \sum_{i,j} d_{ij} |i,j\rangle$, then $|\psi\rangle = |\phi\rangle|\phi'\rangle$ with $|\phi\rangle = \sum_i a_i |i\rangle \in H$ and $|\phi'\rangle = \sum_j b_j |j\rangle \in K$. Thus $d_{ij}=a_ib_j$ and $|\psi\rangle = \sum_{i,j} a_i b_j |i,j\rangle$.

So the density operator is

$$\rho = |\psi\rangle\langle\psi| = \sum_{i,j,i',j'} a_i b_j \overline{a_{i'} b_{j'}}\, |i,j\rangle\langle i',j'|.$$

It follows that

$$\rho^{\text{PHC}} = |\psi\rangle\langle\psi| = \sum_{i,j,i',j'} a_i \overline{b_j a_{i'}} b_{j'}\, |i,j'\rangle\langle i',j|.$$

Note that

$$\rho = |\psi\rangle\langle\psi| = \left(\sum_{i,i'} a_i \overline{a_{i'}} |i\rangle\langle i'|\right) \otimes \left(\sum_{j,j'} b_j \overline{b_{j'}} |j\rangle\langle j'|\right) = \rho_1 \otimes \rho_2$$

and

$$\begin{aligned}\rho^{\text{PHC}} &= \left(\left(\sum_i a_i |i\rangle\right)\otimes\left(\sum_{j'} b_{j'} |j\rangle\right)\right)\left(\left(\sum_{i'} \overline{a_{i'}}\langle i'|\right)\otimes\left(\sum_j \overline{b_j}\langle j|\right)\right)\\ &= \left(\sum_{i,i'} a_i \overline{a_{i'}} |i\rangle\langle i'|\right)\otimes\left(\sum_{j,j'} b_{j'} \overline{b_j} |j'\rangle\langle j|\right)\\ &= \rho_1 \otimes \rho_2 \dagger = \rho_1 \otimes \rho_2.\end{aligned}$$

That is $\rho^{\text{PHC}}=\rho$.

It remains to show that if $\rho^{\text{PHC}}=\rho$, then ρ is separable. If $\rho^{\text{PHC}}=\rho$, we assume that the Schmidt decomposition of $|\psi\rangle$ is $|\psi\rangle = \sum_k \lambda_k |k,k'\rangle$, then

$$\sum_{k,l} \lambda_k \lambda_l |k,k'\rangle\langle l,l'| = \sum_{k,l} \lambda_k \lambda_l |k,l'\rangle\langle l,k'|.$$

It follows that, for any k, l, if $\lambda_k\lambda_l \neq 0$, we have

$$|k,k'\rangle\langle l,l'| = |k,l'\rangle\langle l,k'|.$$

Notice that the above equation is impossible whenever $k \neq l$ and it holds if and only if $k=l=1$. This leads to $|\psi\rangle = |1,1'\rangle$, that is ρ is separable. ■

Remark 1.4. The operation of PHC above is defined by taking the PHC operation on the second subsystem (i.e. K), and the PHC operation with respect to the first subsystem (i.e. H) can also be defined similarly.

Remark 1.5. It seems that there is no natural way to define the PHC operation for mixed states. For any given mixed state $\rho = \sum_i p_i \rho_i$, where $\{\rho_i\}$ is a family of pure states, a natural way to define the PHC of ρ is $\rho^{\text{PHC}} = \sum_i p_i \rho_i^{\text{PHC}}$. However, the representation of ρ is not unique, and above ρ^{PHC} may not be well defined. In [20], Zhao et al. guessed that every mixed separable state is also invariant under PHC. However, the example below shows that this is not the case.

Take

$$\rho_\alpha = \frac{2}{7}|\omega\rangle\langle\omega| + \frac{\alpha}{7}\sigma_+ + \frac{5-\alpha}{7}\sigma_-$$

in a 3×3 system with $\{|0\rangle,|1\rangle,|2\rangle\}$ the orthonormal basis of C^3, i=1, 2, 3, where

$$|\omega\rangle = \frac{1}{\sqrt{3}}(|0,0\rangle + |1,1\rangle + |2,2\rangle),$$

$$\sigma_+ = \frac{1}{3}(|0,1\rangle\langle 0,1| + |1,2\rangle\langle 1,2| + |2,0\rangle\langle 2,0|),$$

$$\sigma_{-}=\frac{1}{3}\left(\left|1,0\right\rangle\left\langle 1,0\right|+\left|2,1\right\rangle\left\langle 2,1\right|+\left|0,2\right\rangle\left\langle 0,2\right|\right)$$

and $2\leqslant\alpha\leqslant 5$. In [26], Horodecki et al. showed that, ρ is separable if and only if $2\leqslant\alpha\leqslant 3$; ρ is entangled if and only if $3<\alpha\leqslant 5$. It is clear that

$$\begin{aligned}\rho_{\alpha}^{\mathrm{PHC}}&=\frac{2}{7}\left|\omega\right\rangle\left\langle\omega\right|^{\mathrm{PHC}}\\&+\frac{\alpha}{21}\left(\left|0,1\right\rangle\left\langle 0,1\right|+\left|1,2\right\rangle\left\langle 1,2\right|+\left|2,0\right\rangle\left\langle 2,0\right|\right)^{\mathrm{PHC}}\\&+\frac{5-\alpha}{21}\left(\left|1,0\right\rangle\left\langle 1,0\right|+\left|2,1\right\rangle\left\langle 2,1\right|+\left|0,2\right\rangle\left\langle 0,2\right|\right)^{\mathrm{PHC}}\\&=\frac{2}{7}\left|\omega\right\rangle\left\langle\omega\right|^{\mathrm{PHC}}\\&+\frac{\alpha}{21}\left(\left|0,1\right\rangle\left\langle 0,1\right|+\left|1,2\right\rangle\left\langle 1,2\right|+\left|2,0\right\rangle\left\langle 2,0\right|\right)\\&+\frac{5-\alpha}{21}\left(\left|1,0\right\rangle\left\langle 1,0\right|+\left|2,1\right\rangle\left\langle 2,1\right|+\left|0,2\right\rangle\left\langle 0,2\right|\right)\\&\neq\rho_{\alpha}\end{aligned}\tag{3}$$

for all $2\leqslant\alpha\leqslant 5$ since $\left|\omega\right\rangle\left\langle\omega\right|$ is a entangled state and, by the PHC criterion, $\left|\omega\right\rangle\left\langle\omega\right|^{\mathrm{PHC}}\neq\left|\omega\right\rangle\left\langle\omega\right|$. As ρ_{α} is separable whenever $2\leqslant\alpha\leqslant 3$, it follows that there exist separable mixed states that are variant under PHC. On the other hand, for any $2\leqslant\alpha\leqslant 3$, as ρ_{α} is separable, there are pure states $\rho_k^{(1)}$, $\rho_k^{(2)}$ and positive numbers $p_k>0$ with $\sum_k p_k=1$, such that

$$\rho_{\alpha}=\sum_k p_k\rho_k^{(1)}\otimes\rho_k^{(2)}.$$

By the PHC criterion, $(\rho_k^{(1)}\otimes\rho_k^{(2)})^{\mathrm{PHC}}=\rho_k^{(1)}\otimes\rho_k^{(2)}$ holds for any k, thus we get that $\rho_{\alpha}^{\mathrm{PHC}}=\rho_{\alpha}$.

Together with eq. (3), we see that the PHC operation for ρ_{α} is not well defined.

Remark 1.6. Just as pointed out in [20], the PHC criterion does not provide us with much convenience, and it only leads us to consider the entanglement problem from a different point of view. In addition, another application of this criterion may be that it can provide a new way to quantify the amount of entanglement of a given state by calculating some distance (such as trace distance) between the given state and the partial hermitian conjugate of the state. However, by Remark 1.5, it can only be used to pure states.

For example, let $\left|\omega\right\rangle=\frac{1}{\sqrt{3}}\left(\left|0,0'\right\rangle+\left|1,1'\right\rangle+\left|2,2'\right\rangle\right)$ and $\left|z\right\rangle=\frac{1}{\sqrt{2}}\left(\left|0,0'\right\rangle+\left|1,1'\right\rangle\right)$ where $\left|0\right\rangle$, $\left|1\right\rangle$, $\left|2\right\rangle$ and $\left|0'\right\rangle$, $\left|1'\right\rangle$, $\left|2'\right\rangle$ are orthonormal sets of H and K, respectively. Then $\rho_{\omega}=\left|\omega\right\rangle\left\langle\omega\right|$ and $\rho_z=\left|z\right\rangle\left\langle z\right|$ are entangled pure states. It is evident that ρ_{ω} is more entangled than ρ_z. Now we consider the trace distance between ρ_{ω} (resp. ρ_z) and $\rho_{\omega}^{\mathrm{PHC}}$ (resp. ρ_z^{PHC}). Observe that $\rho_{\omega}=\frac{1}{3}\left(\left|0,0'\right\rangle\left\langle 0,0'\right|+\left|1,1'\right\rangle\left\langle 1,1'\right|+\left|2,2'\right\rangle\left\langle 2,2'\right|+\left|0,0'\right\rangle\left\langle 1,1'\right|+\left|0,0'\right\rangle\left\langle 2,2'\right|+\left|1,1'\right\rangle\left\langle 0,0'\right|+\left|1,1'\right\rangle\left\langle 2,2'\right|+\left|2,2'\right\rangle\left\langle 0,0'\right|+\left|2,2'\right\rangle\left\langle 1,1'\right|\right)$ and $\rho_{\omega}^{\mathrm{PHC}}=\frac{1}{3}\left(\left|0,0'\right\rangle\left\langle 0,0'\right|+\left|1,1'\right\rangle\left\langle 1,1'\right|+\left|2,2'\right\rangle\left\langle 2,2'\right|+\left|0,1'\right\rangle\left\langle 1,0'\right|+\left|0,2'\right\rangle\left\langle 2,0'\right|+\left|1,0'\right\rangle\left\langle 0,1'\right|+\left|1,2'\right\rangle\left\langle 2,1'\right|+\left|2,0'\right\rangle\left\langle 0,2'\right|+\left|2,1'\right\rangle\left\langle 1,2'\right|\right)$. It follows that the trace distance $D(\rho_{\omega},\rho_{\omega}^{\mathrm{PHC}})$ is

$$D\left(\rho_{\omega},\rho_{\omega}^{\mathrm{PHC}}\right)=\frac{1}{2}\mathrm{Tr}\,|\,\rho_{\omega}-\rho_{\omega}^{\mathrm{PHC}}\,|=\frac{5}{3}.$$

Similarly, we can obtain that

$$D\left(\rho_z,\rho_z^{\mathrm{PHC}}\right)=\frac{1}{2}\mathrm{Tr}\,|\,\rho_z-\rho_z^{\mathrm{PHC}}\,|=1.$$

As desired, we have $D(\rho_{\omega},\rho_{\omega}^{\mathrm{PHC}})>D(\rho_z,\rho_z^{\mathrm{PHC}})$. Thus, it is reasonable to regard the trace distance between ρ and ρ^{PHC} as a measure of entanglement for ρ.

2 Realignment criterion for pure states

For the finite-dimensional case, the realignment criterion [22–24] is a practical criterion that can detect some PPT entangled states [23]. The aim of the present section is to generalize this criterion to infinite-dimensional bipartite quantum systems.

We recall some known facts about the realignment criterion for the finite-dimensional systems. Assume $\dim H=n<\infty$ and $\dim K=m<\infty$ for a moment. In [21], Aniello et al. showed that the (row) realignment of a given pure state can be performed as follows: if $\rho_{\psi}=\left|\psi\right\rangle\left\langle\psi\right|$ is a pure state with $\left|\psi\right\rangle=\sum_{i,j}d_{ij}\left|i,j\right\rangle\in H\otimes K$, let $D=(d_{ij})$ be the $n\times m$ coefficients matrix, and then the (row) realignment of ρ_{ψ} is $\rho_{\psi}^R=D\otimes\overline{D}$.

Inspired by the idea above, we can perform the similar operation on the states in infinite-dimensional bipartite quantum systems. This allows us to generalize the conception of realignment operation to infinite-dimensional case.

Definition 2.1 (Realignment operation). Let H and K be complex Hilbert spaces with orthonormal bases $\{\left|i\right\rangle\}$ and $\{\left|j\right\rangle\}$, respectively. Let $\rho=\left|\psi\right\rangle\left\langle\psi\right|$ be a pure state with $\left|\psi\right\rangle=\sum_{i,j}d_{ij}\left|i,j\right\rangle$. Write $D=(d_{ij})$ and $\overline{D}=(\overline{d_{ij}})$. Then

$$\rho^R=D\otimes\overline{D}$$

is called the realignment operator of ρ. Furthermore, if $\rho=\sum_i p_i\rho_i$ is a mixed state, where $\sum_i p_i=1$, $p_i>0$, ρ_is are pure states. Then $\rho^R=\sum_i p_i\rho_i^R$ is called the realigned operator of ρ.

A similar argument as that for finite-dimensional case [21] shows that the realignment operation is well defined.

The theorem below is the main result of this section which generalizes Proposition 1 in [21] to infinite-dimensional case.

Theorem 2.2 (Realignment criterion). Let $\rho=|\psi\rangle\langle\psi|$ be a pure state in $S(H\otimes K)$ and $|\psi\rangle=\sum_k \lambda_k |k,k'\rangle$ be the Schmidt decomposition of $|\psi\rangle$. Then the realigned operator ρ^R satisfies

$$\|\rho^R\|_{\mathrm{Tr}}=\sum_{i,j}\lambda_i\lambda_j=1+\sum_{i\neq j}\lambda_i\lambda_j\geqslant 1. \tag{4}$$

Moreover,

$$\|\rho^R\|_{\mathrm{Tr}}=1\Leftrightarrow\rho \text{ is separable.} \tag{5}$$

Proof. If $\rho=|\psi\rangle\langle\psi|$, $|\psi\rangle=\sum_{i,j}d_{ij}|i,j\rangle$ and $|\psi\rangle=\sum_k\lambda_k|k,k'\rangle$ is the Schmidt decomposition of $|\psi\rangle$. Let $D=(d_{ij})=U_0D_0V_0$ be the singular value decomposition of D (see eq. (2)), where $D_0=\mathrm{diag}(\lambda_1, \lambda_2, \ldots)$ with $\lambda_1\geqslant\lambda_2\geqslant\ldots$. Then

$$\begin{aligned}\rho_0=D\otimes\overline{D}&=(U_0D_0V_0)\otimes\left(\overline{U_0D_0V_0}\right)\\&=\left(U_0\otimes\overline{U_0}\right)\left(D_0\otimes\overline{D_0}\right)\left(V_0\otimes\overline{V_0}\right).\end{aligned}$$

Let $U=U_0\otimes\overline{U_0}$, $V=V_0\otimes\overline{V_0}$ and $S=D_0\otimes\overline{D_0}$, we have

$$\rho^R=USV.$$

Since $S=D_0\otimes\overline{D_0}$ and $D_0=\mathrm{diag}(\lambda_1, \lambda_2,\cdots)$, we can conclude that, the principal diagonal entries of S are $\{\lambda_i\lambda_j\}$, and therefore

$$\|\rho^R\|_{\mathrm{Tr}}=\sum_{i,j}\lambda_i\lambda_j=1+\sum_{i\neq j}\lambda_i\lambda_j\geqslant 1.$$

The relation (5) is obvious.

Remark 2.3. The realignment criterion is valid for mixed states in infinite-dimensional systems, too. In fact, it is shown in [27] that, for any state $\rho\in S(H\otimes K)$, if ρ is separable, then $\|\rho^R\|_{\mathrm{Tr}}\leqslant 1$.

Theorem 2.2 provides a practical tool to determine whether or not a given pure state is separable since the trace norm of the realignment operator can be calculated easily. In addition, the realignment criterion also implies that the difference $\|\rho^R\|_{\mathrm{Tr}}-\|\rho\|_{\mathrm{Tr}}=\|\rho^R\|_{\mathrm{Tr}}-1$ may be regarded as a measure of entanglement.

3 Some sufficient and necessary conditions of separability for pure states

So far, there are few practical criteria that are both necessary and sufficient for mixed states to be separable [28]. However the situation for pure states is much better. In the previous sections we have proposed two entanglement criteria for pure states in infinite-dimensional systems. In the present section we will give some more criteria of the separability of pure states.

The main result is the following.

Theorem 3.1. Let $|\omega\rangle=\sum_{i,j}d_{ij}|i,j\rangle$ be a unit vector in $H\otimes K$ and $\rho=|\omega\rangle\langle\omega|$. Then the following statements are equivalent: (1) ρ is separable; (2) (The PPT criterion) ρ is PPT; (3) $\|D_\omega\|=1$; (4) there exists a sequence $\{\alpha_j\}$ such that, for some j_0, $d_{ij}=\alpha_j d_{ij_0}$ for all i and $\left(\sum_i|d_{ij_0}|^2\right)\left(\sum_j|\alpha_j|^2\right)=1$; (5) (The PHC criterion) $\rho^{\mathrm{PHC}}=\rho$; (6) (The realignment criterion) $\|\rho^R\|_{\mathrm{Tr}}=1$.

Proof. $(1)\Leftrightarrow(5)$ is proved in Section 1 and $(1)\Leftrightarrow(6)$ is proved in Section 2. Therefore we only need to check the equivalence of (1)–(4). $(1)\Rightarrow(2)$ is obvious.

$(2)\Rightarrow(4)$. For any j, k, let $|x_j\rangle=\sum_{i=1}^\infty d_{ij}|i\rangle\in H$ and $A_{jk}=|x_j\rangle\langle x_k|$. Then

$$\begin{aligned}|\omega\rangle\langle\omega|&=\left(\sum_{ij}d_{ij}|i.j\rangle\right)\left(\sum_{lk}\overline{d_{lk}}\langle l,k|\right)\\&=\sum_{ijlk}d_{ij}\overline{d_{lk}}|i\rangle\langle l|\otimes|j\rangle\langle k|\\&=\sum_{jk}\left(\sum_{il}d_{ij}\overline{d_{lk}}|i\rangle\langle l|\right)\otimes|j\rangle\langle k|\\&=\sum_{jk}|x_j\rangle\langle x_k|\otimes F_{jk}=\sum_{jk}A_{jk}\otimes F_{jk}.\end{aligned}$$

Hence $|\omega\rangle\langle\omega|^{T_1}=\sum_{jk}A_{jk}^T\otimes F_{jk}=\sum_{jk}|x_j\rangle\langle x_k|^T\otimes F_{jk}$ $=\sum_{jk}|\overline{x_k}\rangle\langle\overline{x_j}|\otimes F_{jk}$. It follows that

$$|\omega\rangle\langle\omega| \text{ is PPT } \Leftrightarrow |\omega\rangle\langle\omega|^{T_1}=\sum_{jk}|\overline{x_k}\rangle\langle\overline{x_j}|\otimes F_{jk}\geqslant 0. \tag{6}$$

If $|\omega\rangle\langle\omega|$ is PPT, then, by eq. (6), for any j, k with $j<k$, we have

$$\begin{pmatrix}|\overline{x_j}\rangle\langle\overline{x_j}| & |\overline{x_k}\rangle\langle\overline{x_j}|\\ |\overline{x_j}\rangle\langle\overline{x_k}| & |\overline{x_k}\rangle\langle\overline{x_k}|\end{pmatrix}\geqslant 0.$$

Therefore there exists a contractive operator V_{jk} such that

$$|\overline{x_k}\rangle\langle\overline{x_j}|=\left|\overline{x_j}\rangle\langle\overline{x_j}\right|^{\frac{1}{2}}V_{jk}\left|\overline{x_k}\rangle\langle\overline{x_k}\right|^{\frac{1}{2}}.$$

Due to $\left|\overline{x_j}\rangle\langle\overline{x_j}\right|^{\frac{1}{2}}=\frac{1}{\||x_j\rangle\|}|\overline{x_j}\rangle\langle\overline{x_j}|$ for all j, the above equation yields

$$\left|\overline{x_k}\right\rangle\left\langle\overline{x_j}\right|^{\frac{1}{2}} = \frac{1}{\left\|\left|x_j\right\rangle\right\|\left\|\left|x_k\right\rangle\right\|}\left|\overline{x_j}\right\rangle\left\langle\overline{x_j}\right|V_{jk}\left|\overline{x_k}\right\rangle\left\langle\overline{x_k}\right|$$
$$= \frac{\left\langle\overline{x_j}\right|V_{jk}\left|x_k\right\rangle}{\left\|\left|x_j\right\rangle\right\|\left\|\left|x_k\right\rangle\right\|}\left|\overline{x_j}\right\rangle\left\langle\overline{x_k}\right|.$$

It follows that $\left|\overline{x_k}\right\rangle$ and $\left|\overline{x_j}\right\rangle$ are linearly dependent. As $|\omega\rangle \neq 0$, so $\left|x_{j_0}\right\rangle \neq 0$ for some j_0. Thus, there exists scalar α_k such that $\left|x_k\right\rangle = \alpha_k\left|x_{j_0}\right\rangle$. Particularly, for any k, $\left|\overline{x_k}\right\rangle$ and $\left|\overline{x_{j_0}}\right\rangle$ are linearly dependent, that is, $\left|x_k\right\rangle$ and $\left|x_{j_0}\right\rangle$ are linearly dependent. Therefore for any i and k>1, we get $d_{ik} = \alpha_k d_{ij_0}$. Note that $\left\||\omega\rangle\right\| = 1$ and

$$\langle\omega|\omega\rangle = \sum_{ij} d_{ij}\langle i,j|\sum_{lk} d_{lk}\, l,k\rangle$$
$$= \sum_{i,j,l,k} d_{ij}\overline{d_{lk}}\langle i,j|l,k\rangle = \sum_{i,j}\left|d_{ij}\right|^2.$$

This implies $\left(\sum_i\left|d_{ij_0}\right|^2\right)\left(\sum_j\left|\alpha_j\right|^2\right) = 1$.

$(4)\Rightarrow(1)$. Without loss of generality, we assume that $d_{ij} = \alpha_j d_{i1}$ for all i, j with j>1 and thus $\left(\sum_i\left|d_{i1}\right|^2\right)\left(\sum_i\left|d_{i1}\right|^2\right) = 1$. By the definition of $\left|x_j\right\rangle$, we get $\left|x_j\right\rangle = \alpha_j\left|x_1\right\rangle$. Let $|x\rangle = \frac{1}{\sum_i\left|d_{i1}\right|^2}\left|x_1\right\rangle$ and $|y\rangle = \frac{1}{\Sigma_j\left|a_j\right|^2} \times\sum_j \alpha_j\,|j\rangle$. Then

$$|\omega\rangle\langle\omega| = \sum_{jk}\alpha_j\overline{\alpha_k}\left|x_1\right\rangle\left\langle x_1\right|\otimes|j\rangle\langle k|$$
$$= |x\rangle\langle x|\otimes|y\rangle\langle y|.$$

Therefore ρ is separable.

$(4)\Rightarrow(3)$. (4) implies that $D_\omega = \left(d_{ij}\right)$ is of rank one. Hence $\left\|D_\omega\right\| = \left\|D_\omega\right\|_2 = \left\||\omega\rangle\right\|^2 = 1$.

$(3)\Rightarrow(4)$. $\left\|D_\omega\right\| = 1$ implies that $\left\|D_\omega\right\| = \left\|D_\omega\right\|_2$. Therefore D_ω is of rank one and thus (4) holds. ■

Next, we give a proposition related to the item (3) of Theorem 3.1. Before doing this we recall some known facts. In [28,29], the so-called entanglement witness criterion was proposed. It was shown that, a state ρ (in finite- or infinite-dimensional systems) is entangled if and only if there exists an observable W of the composite system such that Tr($W\rho$)<0, where W satisfying Tr($W\sigma$)⩾0 for all separable states σ. Based on this criterion, together with the fact that $\left\|D_\omega\right\| \leqslant 1$ holds for any unit vector $|\omega\rangle \in H\otimes K$, we can conclude that $\rho = |\omega\rangle\langle\omega|$ is entangled if and only if $\left\|D_\omega\right\| < 1$ by Theorem 3.1, item (3). Indeed, a little more can be said.

Proposition 3.2. Let $\rho = |\omega\rangle\langle\omega|$ with $|\omega\rangle = \sum_{i,j} d_{ij}|i,j\rangle \in H\otimes K$ be a pure state and regard D=(d_{ij}) as an operator from K into H. Then $W = \|D\|^2 I - \rho$ satisfies Tr($W\sigma$)⩾0 for all $\sigma \in S_0$. Moreover, ρ is entangled if and only if $\|D\| < 1$. In this case, W is an entanglement witness of ρ.

Proof. Let $|\mu\rangle = \sum_i a_i|i\rangle$ with $\sum_i\left|a_i\right|^2 = 1$ and $|\upsilon\rangle = \sum_j b_j|j\rangle$ with $\sum_j\left|b_j\right|^2 = 1$. Then

$$\left|\langle\omega|\mu,\upsilon\rangle\right| = \left|\sum_{i,j}\overline{d_{ij}}\langle i,j|\sum_{i',j'} a_{i'}b_{j'}|i',j'\rangle\right|$$
$$= \left|\sum_{i,j}\overline{d_{ij}}a_i b_j\right| = \left|\sum_i a_i\left(\sum_j\overline{d_{ij}}b_j\right)\right|$$
$$= \left|\left\langle\overline{\mu}\right|\overline{D}|\nu\rangle\right|,$$

where $\overline{D} = (\overline{d_{ij}})$ and $\left|\overline{\mu}\right\rangle = \overline{|\mu\rangle}$. Thus we get

$$\sup_{\sigma\in S_0}\left|\mathrm{Tr}\left(|\omega\rangle\langle\omega|\sigma\right)\right| = \sup_{\||\mu\rangle\|=1,\||\nu\rangle\|=1}\left|\langle\omega|\mu,\nu\rangle\right|^2 = \|D\|^2. \quad (7)$$

Let $A = \|D\|^2 I - |\omega\rangle\langle\omega|$. It is clear that Tr($W\sigma$)⩾0 for all separable pure state $\sigma \in S_0$. If $\|D\|^2 < 1$, then Tr($A\rho$)= $\|D\|^2 - \mathrm{Tr}\left(\rho^2\right) = \|D\|^2 - 1 < 0$. Hence ρ is entangled and W is an entanglement witness of ρ. ■

At last, we give an example of the application of the criteria.

Example 3.3. Let $\rho = |\psi\rangle\langle\psi| \in S$ with $|\psi\rangle = \frac{1}{3}\left(|0,0'\rangle + |0,1'\rangle - i|0,2'\rangle + |1,0'\rangle + |1,1'\rangle - i|1,2'\rangle + i|2,0'\rangle + i|2,1'\rangle + |2,2'\rangle\right)$, where $|0\rangle$, $|1\rangle$, $|2\rangle$ and $|0'\rangle$, $|1'\rangle$, $|2'\rangle$ are orthonormal sets of H and K, respectively. It is clear that

$$D_\psi = \tfrac{1}{3}\begin{pmatrix} 1 & 1 & -i & 0 & \cdots \\ 1 & 1 & -i & 0 & \cdots \\ i & i & 1 & 0 & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

By calculating, we can obtain that (1) $\rho^{T_2} \geqslant 0$ (equivalently, $\rho^{T_1} \geqslant 0$); (2) $\rho^{\mathrm{PHC}} = \rho$; (3) $\|D\| = 1$; (4) Take j_0=3 and $\alpha_1 = \alpha_2 = i$, $\alpha_3 = 1$, we have $d_{ij} = \alpha_j d_{i3}$ and $\left(\sum_i\left|d_{i3}\right|^2\right)\left(\sum_j\left|\alpha_j\right|^2\right) = 1$; (5) $\left\|\rho^R\right\|_{\mathrm{Tr}} = 1$. Therefore by Theorem 3.1, ρ is separable.

In conclusion, we have given several sufficient and necessary conditions of separability for pure states in infinite-dimensional bipartite systems which provide some principal insights into the structure of the pure states. Some conditions provide tools to study the entanglement measures on the set of pure states.

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