Positive Maps Which Are Not Completely Positive

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The concept of the half density matrix is proposed. It unifies the quantum states which are described by density matrices and physical processes which are described by completely positive maps. With the help of the half-density-matrix representation of Hermitian linear maps, we show that every positive map which is not completely positive is a difference of two completely positive maps. A necessary and sufficient condition for a positive map which is not completely positive is also presented, which is illustrated by some examples.

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Entanglement has become one of the central concepts in quantum mechanics, especially in quantum information. A quantum state of a bipartite system is entangled if it cannot be prepared locally or it cannot be expressed as a convex combination of direct product states of two subsystems. This kind of state is also called inseparable. Though easily defined, it is very hard to recognize the inseparability of a mixed state of a bipartite system.

An operational-friendly criterion of separability was proposed by Peres [1]. This criterion is based on the observation that the partial transposition of a separable density matrix remains positive semidefinite. That the partial transposition of a density matrix is not positive semidefinite infers the inseparability of the density matrix. This provides a necessary condition for the separability. There exist entangled states with positive partial transposition, which exhibit bound entanglement [3]. Examples of such kind were first provided in Ref. [3] and then constructed in Ref. [4] systematically with the help of unextendible product basis.

Later on, by noticing that the transposition is a positive map (to be described later in details), a necessary and sufficient condition of the separability was proposed in Ref. [5]: A bipartite state is separable iff it is still positive semidefinite under all positive maps acting on a subsystem. In other words, a density matrix of a bipartite system is inseparable iff there exists a positive map acting on a subsystem such that the image of the density matrix is not positive semidefinite. Hence the inseparability can be recognized by positive maps which are not completely positive.

Completely positive maps, which are able to describe the most general physical process [6], are better understood than positive maps which are not completely positive. Positive maps from Hilbert space \(\mathcal{H}_2\) (two-dimensional) to \(\mathcal{H}_2\) or \(\mathcal{H}_3\) are all decomposable [6], which are characterized by transposition and completely positive maps only. As a result in the cases of \(\mathcal{H}_2 \times \mathcal{H}_2\) and \(\mathcal{H}_2 \times \mathcal{H}_3\) the transposition criterion is also a sufficient condition for separability [6]. Therefore further understandings of positive maps which are not completely positive will facilitate the recognition and classification of the inseparable mixed states.

As a direct calculation will show, under an orthonormal and complete basis \(\{ |n\rangle \}_{n=0}^{L-1}\) the transposition of an \(L \times L\) matrix \(\rho\) can be expressed as

\[
\rho^T = \text{Tr}(\rho) - \sum_{m,n=0}^{L-1} \sigma_{mn} \rho \sigma_{mn}^T,
\]

where \(\sigma_{mn} = (|m\rangle \langle n| - |n\rangle \langle m|)/\sqrt{2}\). We see immediately that the transposition is a difference of two completely positive maps. And this statement will be proved to hold true for all positive maps which are not completely positive, which will be also characterized by a necessary and sufficient condition in this Letter.

For this purpose we shall first develop an extremely useful tool — half density matrix that unifies the description of the quantum states and physical processes. And then we derive a half-density-matrix representation of an arbitrary Hermitian linear map from which our main results are obtained. Along with the introduction of the concept of half density matrix, its relations to the ensembles and the purifications of mixed states are clarified and its applications in the field of quantum information such as quantum teleportation [6] are also presented.

Normally, quantum states, pure or mixed, are described by density matrices, positive semidefinite operators (whose eigenvalues are all nonnegative) on the Hilbert space of the system. Because of its property of positive semidefinite the density matrix \(\rho\) can always be written as \(\rho = TT^\dagger\) where matrix \(T\) is called here as the half density matrix (HDM) for a quantum state.

Obviously, the half density matrix for a given density matrix is not unique. For example \(TU\) and \(T\) are corresponding to the same mixed state \(\rho = TT^\dagger\) whenever \(U\) is unitary. Generally, the half density matrix \(T\) for a mixed state \(\rho\) of an \(s\)-level system is an \(s \times L\) rectangular matrix with \(L \geq r = \text{Rank} (\rho)\), i.e., a linear map from an \(L\)-dimensional Hilbert space \(\mathcal{H}_L\) to an \(s\)-dimensional Hilbert space \(\mathcal{H}_s\). The rank \(r\) of the density matrix equals to the rank of the half density matrix \(T\) and \(r = 1\) for pure state.

Under an orthonormal and complete bases \(\{|m\rangle\}_{m=0}^{s-1}\) and \(\{|n\rangle\}_{n=0}^{L-1}\) of Hilbert spaces \(\mathcal{H}_s\) and \(\mathcal{H}_L\), a typical half density matrix of dimension \(s \times L\) can be constructed as \(T = \sqrt{\Delta} V (\Delta, \mathbf{0}, \mathbf{L}_{s-L})\), where \(\Delta\) is a diagonal \(s \times s\) matrix formed by all the square roots of the eigenvalues of \(\rho\) (the singular numbers of \(T_L\)) and \(V\) is an \(s \times s\) unitary matrix diagonalizing the density matrix \(\rho\). Obviously we have \(\rho = T T^\dagger\). As a direct result of the singular number decomposition of an arbitrary matrix [6] we have the following...
Lemma: Given a density matrix $\rho$ of an $s$-level system, an $s \times L$ matrix $T$ is a half density matrix for $\rho$, i.e., $\rho = TT^\dagger$, if and only if there exists an $L \times L$ unitary matrix $U$ such that $T = TU$. When written explicitly in the established basis, the relation $\rho = T\rho T^\dagger$ results in exactly an ensemble formed by all the eigenvectors $V_m$ of the mixed state, which is referred to as the eigen-ensemble here. In this way every half density matrix $T$ of a mixed state $\rho$ corresponds to an ensemble of the mixed state. The above lemma tells us that every ensemble of a given mixed state is related to the eigen-ensemble by a unitary matrix which has been proved by other means [11]. Therefore the half density matrix of a density matrix is physically equivalent to a system $sL$ as the corresponding mixed state.

Every mixed state $\rho$ admits a purification [13]; a pure state $|\phi\rangle$ of a bipartite system including this system as a subsystem such that $\rho = \text{Tr}_2|\phi\rangle\langle\phi|$ Under the established basis, a general pure state in $sL \otimes H_L$ is

$$|\phi\rangle = \sum_{m=0}^{s-1} \sum_{n=0}^{L-1} C_{mn} |m\rangle_1 |n\rangle_2 := T|\Phi_L\rangle.$$

Here pure state $|\Phi_L\rangle = \sum_{m=0}^{s-1} |m\rangle_1 |n\rangle_2$ lives in Hilbert space $H_L \otimes H_L$, and $T$ is a linear map from $H_L$ to $H_s$ acting on the first $L$-dimensional Hilbert space $H_L$. Under the given bases linear map $T$ is represented by an $s \times L$ rectangular matrix with matrix elements given by $|m\rangle T |n\rangle = C_{mn}$. When the pure state $|\phi\rangle$ is normalized we have $\text{Tr}(T^\dagger T) = 1$. Alternatively, we also have $|\phi\rangle = T^\dagger |\Phi_s\rangle$ with state $|\Phi_s\rangle$ defined in $H_s \otimes H_s$ similar to state $|\Phi_L\rangle$. The linear map $T^\dagger : H_s \otimes H_L \rightarrow H_L$ acts on the second $H_s$ and it is represented by the transposition of $T$ under the established basis.

Tracing out the second system we obtain a reduced density matrix of the first subsystem $\rho_s = TT^\dagger$ and similarly $\rho_L = TT^\dagger$ for the second subsystem. That is to say $T$ is the EDM for the reduced half density matrix $\rho_s = \text{Tr}_2|\phi\rangle\langle\phi|$ of the first subsystem and its transposition $T^\dagger$ for $\rho_L = \text{Tr}_s|\phi\rangle\langle\phi|$. Thus a one-to-one correspondence between a normalized pure state $|\phi\rangle$ of a bipartite system, a purification, and a linear map $T$ satisfying $\text{Tr}(T^\dagger T) = 1$, a half density matrix, is established. Therefore a half density matrix $T$ is also equivalent to a purification of the mixed state. The linear map $T$ is also referred to as the half density matrix of a bipartite pure state, which is unique by definition. If $s = L$ the polar decomposition of $T$ will result in the useful Schmidt-decomposition.

The pure bipartite state is separable iff the rank of its half density matrix is one. For a pure product state $|\psi\rangle_1 |\psi\rangle_2$ the half density matrix is $|\psi\rangle_1 \langle w| \langle \psi|_2$ where $w$ is the index state of state $|\psi\rangle$ defined by $|\psi\rangle = (w|_2 \Phi_1) \Phi_1$. For later use we define a mirror operator $M_L = |\Phi_L\rangle\langle \Phi_L|$ in the Hilbert space $H_s \otimes H_L$, which has the property $(w^* |_2 M_L |w) = (w|_2 \Phi_1)$. The partial transposition of the mirror operator $X = M_L^\dagger$ is in fact the exchanging (or swapping) operator introduced by Werner [13] (denoted as $V$ there).

As an application, we consider a state $|\phi\rangle_1 |\psi\rangle_3$ of a tripartite system with all three subsystems 1, 2 and 3 being $s$-level systems. Let $T_3$ denote the EDM of the bipartite state $|\phi\rangle_{12}$ and $|k;l\rangle_{23} = T_{kl} |\Phi_{23}\rangle$ denote an orthonormal complete basis for systems 2 and 3 with EDMs $T_{kl}$ satisfying $\text{Tr} T_{kl} T_{kl}^\dagger = \delta_{k,k'} \delta_{l,l'}$ for orthogonality and $\sum_{kl} T_{kl} \text{Tr} T_{kl}^\dagger = \text{Tr} O$ for completeness. We then have expansion

$$|\phi\rangle_{12} |\psi\rangle_3 = \sum_{k,l=0}^{s-1} T_{kl} T_{kl}^\dagger |\psi\rangle_1 |k;l\rangle_{23}.$$

This describes exactly a quantum teleportation of an unknown quantum state $|\psi\rangle$ from system 3 to system 1 when both $T_\phi$ and $T_{kl}$ are unitary or state $|\phi\rangle_{12}$ and basis $|k;l\rangle_{23}$ are maximally entangled states [13].

The mixed state $\rho_{sL}$ of an $(s \times L)$ bipartite state can also be equivalently and conveniently characterized by EDM's of pure bipartite states. Let $\{ |\phi_i\rangle, p_i \}_{i=1}^R$ be an ensemble of $\rho_{sL}$ we have

$$\rho_{sL} = \sum_{i=1}^R p_i |\phi_i\rangle \langle \phi_i|.$$

where we have denoted $A_i$ as the half density matrix of the pure state $\sqrt{p_i} |\phi_i\rangle$, i.e., $\sqrt{p_i} |\phi_i\rangle = A_i |\Phi_L\rangle$. Obviously EDM's defined by $A_i = \sum_j U_{ij} A_j$ characterize the same density matrix whenever $U$ is a unitary matrix. And from the Lemma we know that given a density matrix this is the only freedom that the half density matrices can have.

The density matrix expressed in the form as in Eq. (4) can be easily manipulated by local operations. For example the density matrix under operation $U_s \otimes U_L^\dagger$ is transformed to density matrix specified by half density matrices $U_s A_j U_L^\dagger$. The tilde operation $\rho \mapsto \tilde{\rho}$ introduced in Ref. [14] to obtain explicitly the entanglement of formation of two-qubit is simply an antilinear transformation $A_i \mapsto A_i^* - A_i$.

In the discussions above we have defined the half density matrices for the states of a single system, for pure bipartite states, and for mixed bipartite states. The physical processes can also be characterized by half density matrices. A general physical process which can include unitary evolutions, tracing out one system, and general measurements is described by trace-preserving completely positive maps [6, 11], which is a special kind of Hermitian linear map.

A Hermitian linear map sends linearly Hermitian operators to Hermitian operators that may live in different Hilbert spaces. Let $L$ denote a general Hermitian linear map from Hilbert space $H_L$ to $H_s$. Because the map $L$ is linear the map $L \otimes L_L$ is also a Hermitian linear map from $H_s \otimes H_L$ to $H_s \otimes H_L$, where $L_L$ denotes the identity map on $H_L$. Recalling that the mirror operator $M_L = |\Phi_L\rangle\langle \Phi_L|$ is defined on $H_s \otimes H_L$, its image

$$H_{sL} = L \otimes L_L (M_L)$$

is therefore a Hermitian operator in $H_s \otimes H_L$. Let $|\psi_i\rangle = A_i |\Phi_L\rangle$ ($i \leq i_+$) denote the eigenvectors corresponding to the positive eigenvalues of $H_{sL}$ and $|\psi_i\rangle = B_i |\Phi_L\rangle$ ($i \leq i_-$) to negative eigenvalues of $H_{sL}$, where $i_\pm$ is the number of the
positive/negative eigenvalues of $H_{sL}$. We then have
\[ H_{sL} = \sum_{i=1}^{i_+} A_i M_L A_i^\dagger - \sum_{i=1}^{i_-} B_i M_L B_i^\dagger, \tag{6} \]
in which the norms of the eigenvectors $|\psi_i^\pm\rangle$ have been taken to be the absolute values of corresponding eigenvalues. Because the eigenvectors corresponding to different eigenvalues are orthonormal we have $\text{Tr}(A_i B_j^\dagger) = 0$ for all $i$ and $j$. In this sense two families of half density matrices $\{A_i\}$ and $\{B_i\}$ are orthogonal to each other.

For a pure state $P_w = |w\rangle\langle w|$ in the Hilbert space $\mathcal{H}_L$ we have $P_w = \langle w^* | M_L | w^* \rangle$ where $|w^*\rangle$ is the index state of $|w\rangle$. As a result we have $\mathcal{L}(P_w) = \langle w^* | H_{sL} | w^* \rangle$. Taking into account of the linearity of the Hermitian map $\mathcal{L}$, we finally obtain
\[ \mathcal{L}(H) = \sum_{i=1}^{i_+} A_i H A_i^\dagger - \sum_{i=1}^{i_-} B_i H B_i^\dagger, \tag{7} \]
where $H$ is an arbitrary Hermitian matrix in $\mathcal{H}_L$. This is called the half-density-matrix representation of a Hermitian linear map. As one result we have
\[ \langle \Phi_s | I_s \otimes \mathcal{L}(\Sigma_{sL}) | \Phi_s \rangle = \text{Tr}(H_{sL} \Sigma_{sL}^T) \tag{8} \]
for an arbitrary Hermitian matrix $\Sigma_{sL}$ in $\mathcal{H}_s \otimes \mathcal{H}_L$. As another consequence, a one-to-one correspondence between the Hermitian maps $\mathcal{L} : \mathcal{H}_L \mapsto \mathcal{H}_s$ and Hermitian matrix $H_{sL}$ (an observable) in $\mathcal{H}_s \otimes \mathcal{H}_L$ can be established
\[ \mathcal{L}(H) = \text{Tr}_L(H_{sL} H^T) \tag{9} \]
in addition to Eq.\([5\]).

The HDM representation of Hermitian linear map is not unique. Suppose two integers $M \geq i_+$ and $N \geq i_-$ and let $SU(M,N)$ denote the pseudo-unitary group formed by $(M + N) \times (M + N)$ matrices satisfying $S \eta S^\dagger = \eta$ where $\eta = I_M \oplus (-I_N)$ and $I_{M+N}$ is the $M \times M$ matrix ($N \times N$) identity matrix. If we define a family of HDMs $\{T_i\}_{i=1}^{M+N}$ as $T_i = A_i$ (1 $\leq i \leq i_+$), $T_i = B_i$ ($M + 1 \leq i \leq M + i_-$) and $T_i = 0$ otherwise and take an arbitrary element $S$ of $SU(M,N)$, a new family of HDMs $\{T_i\}_{i=1}^{M+N}$ defined by $\tilde{T}_i = \sum_j S_{ij} T_j$ represents the same Hermitian linear map
\[ \mathcal{L}(H) = \sum_{i=1}^{M} \tilde{T}_i H \tilde{T}_i^\dagger - \sum_{j=1}^{N} \tilde{T}_j H^T \tilde{T}_j^\dagger, \tag{10} \]
for a Hermitian linear map $\mathcal{L} : \mathcal{H}_L \mapsto \mathcal{H}_s$ and an arbitrary positive integer $k$ the induced map $\mathcal{S} \otimes I_k$ from $\mathcal{H}_L \otimes \mathcal{H}_k$ to $\mathcal{H}_s \otimes \mathcal{H}_k$ is positive.

However it is enough to check whether the image $H_{sL} = \mathcal{S} \otimes I_L(M_L)$ of the mirror operator $M_L$ is positive semidefinite or not. If it is positive semidefinite, then the negative part in the HDM representation Eq.\([3\]) disappears, which yields exactly the operator-sum representation of a CP map \[ S(\rho) = \sum_{i=1}^{i_+} A_i \rho A_i^\dagger. \tag{11} \]

If the trace is preserved, we have further $\sum_i A_i^\dagger A_i = 1$. Therefore the operator-sum representation of a CP map can also be referred to as a half-density-matrix representation. Especially, if $H_{sL}$ equals to the identity matrix $I_s \otimes I_L$, the corresponding CP map is simply the trace operation $S_T(\rho) = I_s \text{Tr}_p$.

A positive map which is not completely positive (non-CP) is nonetheless a Hermitian map so that it has a HDM representation as Eq.\([4\]) from which we obtain $S = S_A - S_B$ where two CP maps $S_{A,B}$ are represented by HDMs $\{A_i\}$ and $\{B_i\}$ respectively. Two CP maps $S_{A,B}$ are said to be orthogonal if their HDMs are orthogonal to each other, i.e., $\text{Tr}(A_i B_j^\dagger) = 0$ for all $i, j$. We see that $H_{sL}$ can not be positive semidefinite.

Conversely, if the Hermitian matrix $H_{sL}$ has at least one negative eigenvalue then it determines a non-CP positive map. Let $|\psi\rangle$ denote an eigenvector corresponding to one of the negative eigenvalues of $H_{sL}$ and $P_\psi = |\psi\rangle \langle \psi |$. From identity \([8\]) we see immediately that $I_s \otimes S(P_\psi^\dagger)$ is not positive semidefinite, i.e., map $S$ is not completely positive. We note that the eigenspace corresponding to the negative eigenvalues of $H_{sL}$ contains no product state because of positivity. To summarize, we have the following

**Theorem:** Every positive map which is not completely positive is a difference of two orthogonal completely positive maps: A Hermitian linear map $S : \mathcal{H}_L \mapsto \mathcal{H}_s$ is positive but not completely positive if and only if for all pure product state $P_s \otimes Q_L$ in $\mathcal{H}_s \otimes \mathcal{H}_L$ we have $\text{Tr}(H_{sL} P_s \otimes Q_L) \geq 0$ while $H_{sL} = \mathcal{S} \otimes I_L(M_L)$ is not positive semidefinite.

This theorem provides an obvious way to construct a non-CP positive map form $\mathcal{H}_L$ to $\mathcal{H}_s$. First, we choose a proper Hermitian matrix $H_{sL}$ in $\mathcal{H}_s \otimes \mathcal{H}_L$ satisfying the conditions specified in the above theorem. Then a non-CP positive map $S : \mathcal{H}_L \mapsto \mathcal{H}_s$ is determined by $S(\rho_L) = \text{Tr}_L(H_{sL} \rho_L^T)$.

As the first example we consider the the exchanging operator defined in $\mathcal{H}_L \otimes \mathcal{H}_L$ by $X = M_L^T$ or explicitly
\[ X = \sum_{m,n=0}^{L-1} |m,n\rangle\langle n,m|, \tag{12} \]

The exchanging operator $X$ has two eigenvalues $\pm 1$ and $s_{mn}|\Phi_L\rangle$ $(n > m)$ are the eigenvectors corresponding to eigenvalue $-1$. Therefore $X$ is not positive semidefinite and for any pure product states $|pp\rangle = |v\rangle |w\rangle$ we have $\langle pp|X|pp\rangle = |\langle v|w\rangle|^2 \geq 0$ as specified by the above theorem. In fact the resulting non-CP positive map on $\mathcal{H}_L$ is exactly the transposition $\rho^T = \text{Tr}_2(X \rho^T)$. By writing $X$ in its diagonal
form we obtain \( \rho^T = S_T(\rho) - S_s(\rho) \), where the CP map \( S_s \) is represented by HDMs \( \{\sigma_{mn}\} \) and \( S_T \) is the trace operation.

As the second example we consider a Hermitian matrix in \( \mathcal{H}_L \otimes \mathcal{H}_L \) defined by \( H_R = I_L \otimes I_L - M_L \). It is not positive semidefinite because \( \langle \Phi_L | H_R | \Phi_L \rangle < 0 \) and for every product states \( |pp\rangle \) we have \( \langle pp | H_R | pp \rangle = 1 - |\langle v | w^* \rangle|^2 \geq 0 \). Accordingly, a non-CP positive map is defined on \( \mathcal{H}_L \) as \( \Lambda(\rho) = Tr_H \rho \) which provides the reduction criterion \[15, 16\]: Every inseparable state in \( \mathcal{H}_L \otimes \mathcal{H}_L \) which loses its positivity under map \( I_L \otimes \Lambda \) is distillable and in the distillation procedure provided in Ref. \[13\] the HDM of pure bipartite state serves as the filtering operation. Because \( \Lambda(\rho) = S_s(\rho^T) \), the reduction map \( \Lambda \) is a decomposable positive map, which is generally of form \( S_d(\rho) = S_1(\rho) + S_2(\rho^T) \) with \( S_1, S_2 \) being two CP maps.

The last example makes use of an unextendible product basis \[1\]. A set of orthonormal product basis \( \{ |\alpha_i \rangle |\beta_i \rangle \} \) of \( \mathcal{H}_S \otimes \mathcal{H}_L \) where \( S < s L \) and there is no other pure product state that is orthogonal to this set of basis. If we denote \( P = \sum |\alpha_i \rangle \langle \alpha_i | \otimes |\beta_i \rangle \langle \beta_i | \) then \( \tilde{\rho} = (1 - P)/(s L - S) \) represents an inseparable states with positive partial transposition. If we define

\[
\epsilon = \min_{|\alpha| |\beta|} \langle \alpha | \beta | P | \alpha \rangle |\beta \rangle
\]

it can be sure that \( 0 < \epsilon \leq S/s L \) \[17\]. Denoting \( \rho_0 \) as a normalized density matrix in \( \mathcal{H}_S \otimes \mathcal{H}_L \) which has the property \( Tr(\rho_0 \tilde{\rho}) > 0 \), we define a Hermitian matrix as \( H_e = P - \epsilon d \rho_0 \) where

\[
\frac{1}{d} = \max_{|\alpha| |\beta|} \langle \alpha | \beta | \rho_0 | \alpha \rangle |\beta \rangle
\]