Generalized marginal problem in terms of multi-system Hermitian and positive semidefinite matrices

Ruoli Bai

Arcadia High School, Arcadia,California, 91007, United States;

Abstract. We study the reduction from a bipartite Hermitian matrix H to two single-qubit reduced Hermitian matrices HA and HB and the inverse problem. The inverse problem extends the so-called marginal problem from quantum information theory. We explicitly obtain the expressions of the matrices mentioned above and then extend them to positive semidefinite matrices by showing several inequalities involving a few parameters from the matrices. We also extend our results to multi-quit matrices. Our study constructs the intimate connection between the generalized marginal problems in terms of Hermitian matrices and the traditional marginal problem in terms of positive semidefinite matrices.

Keywords: Marginal problem; Two-qubit system; Hermitian matrix; Positive semidefinite matrix.

1. Introduction

Due to the large number of data in the real world, people always hope to find useful information and facts by reading only a part of the target they need to learn [1]Such a problem has been named the so-called marginal problem in quantum chemistry[2,3] since the middle of the last century. The problem has been introduced and studied in quantum physics and the information community for around 30 years. The progress is small, mainly due to the difficulty of mathematics in characterization between the so-called reduced density operators and global density operators. For example, one hopes to use quantum tomography to re-establish the global state with few measurement results on single-system density operators [4].Researchers have also presented the so-called quantum science technology (QST) to show an effective approach to studying the state of many systems such as basic science research, materials science and drug development[5,6].

The unique feature of marginal problems is essential in the efficient QST[5,7,8]. For example, one may consider the marginal problem from a pure state (a multiple tensor in linear algebra and tensor analysis) with identical reduced states[9]. Certainly, the problem examines two scenarios: one where no other pure state meets the required criterion[10] and another where no additional state fulfills the desired requirement. These research works are motivated by practical purposes such as tomography and unique ground states for cooling down[11,12] and a hierarchy of topological order[13,14].

On the other hand, researchers often construct the so-called stabilizer codes using graphs of large-number systems, which can be understood using their reduced systems[15]. From a mathematical point of view, whether the single-party reductions can determine bipartite states or matrices is an interesting problem in that the number of parameters is usually large[9,16,17]. Research has indicated that only two bipartite reduced states can uniquely identify the overwhelming majority of tripartite pure states when considering a pure state. Similar facts have been established in some tripartite systems of higher dimensions[18,19].

In this paper, we extend the marginal problem to the case of mapping a bipartite Hermitian matrix to two single-system Hermitian matrices. Then we ask the converse problem. We explicitly construct the expressions of Hermitian matrices and study the subscales when they become two-qubit positive semidefinite matrices. Our study shows that by choosing some parameters involved in the matrices, one may find some intervals by which the original matrices remain positive semidefinite.

2. Preliminaries

2.1 Complex numbers and linear algebra basics

We denote $M_{n,n} = M_n$, which means the set of order-n matrices. Besides, we apply the formula $\bar{r}=e^{i\theta} * r$, and we have $r*(\cos\theta + i\sin\theta)$, and find that when the value of θ between 0 and 2π, then we have an equation $\bar{r}=r\cos\theta+ir\sin\theta$. The right side of this equation is expressed as a complex number, which includes the term representing the real portion, $r\cos\theta$, and the term for the imaginary portion, $r\sin\theta$.

If $x \in C^n$, then $x=\begin{pmatrix} x_1 \\ \vdots \\ \vdots \\ x_n \end{pmatrix} \in C^n \supset R^n$, R^n is a subspace of C^n, and x is a unit vector if and only if $\sum_{j=1}^{n} |x_j|^2=1$. We know that elements of a linear space are vectors, and C^n means n-dimensional Hilbert space, generally $n < +\infty$, sometimes $n \le +\infty$. R_n means n-dimensional Euclidean space, also named finite dimension, $n < +\infty$.

The number $xa + yb$ can be any linear combination and all $x, y \in C$. 2. satisfy commutative law, associative law, and so on.

Definition 2.1.1. The trace of a matrix A of size n×n, denoted as Tr(A), represents the sum of its diagonal entries, which can be expressed as $\mathrm{Tr}(A)=\sum_{i=1}^{n} a_{ii}$.

For example, $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ is an order-2 orthogonal matrix because the transpose matrix of this matrix is $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$. We know that $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}=I_n$, so this matrix is an order-2 orthogonal

matrix. If $A, B \in O_n(R)$, then we have $AB \in O_n(R)$, the proof is following,

$$(AB) \times (AB)^T = ABB^TA^T = AA^T = I_n,$$

So $AB \in O_n(R)$. We know that the orthogonal matrix set is closed under matrix multiplication. Besides, the symmetric matrix satisfies $A = A^T$, and the anti-symmetric matrix satisfies $A = -A^T$.

2.2 Kronecker Product

Claim 2.2.1. If matrix A and B satisfy $A \otimes B = B \otimes A$, we can conclude sA = kB, where s and k are constants, or scalars, and $k, s \in C$.

First, we have
$$B\otimes A=\begin{pmatrix} b_{1,1}A & b_{1,2}A & \dots & b_{1,q}A \\ b_{2,1}A & b_{2,2}A & \dots & b_{2,q}A \\ \vdots & \vdots & \vdots & \vdots \\ b_{m,1}A & b_{m,2}A & \dots & b_{m,q}A \end{pmatrix}, \tag{1}$$

So we set an order-n matrix F_n and an order-m matrix F_m:

$$F_n=\begin{pmatrix} 1 & \dots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \dots & 1 \end{pmatrix}, F_m=\begin{pmatrix} 1 & \dots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \dots & 1 \end{pmatrix}. \tag{2}$$

For $F_n \otimes F_m$, we obtain an order-mn matrix, and all the elements are 1. We obtain an order-mn matrix for $F_n \otimes F_m$, and all the elements are also one. So we have $F_n \otimes F_m = F_m \otimes F_n$. If m and n are positive integers, there will be an infinite number of values of m and n, so we cannot have A and B as homomorphic matrices, and we cannot have any special relationships from this equation.

2.3 Positive semidefinite matrix

Definition 2.3.1. We have a Hermitian matrix $H=U^{*}\begin{pmatrix} d_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & d_n \end{pmatrix}U$. If $d_j \geq 0$, then we say that H is positive semidefinite.

A positive semidefinite matrix of trace one is a quantum state/ density operator in quantum physics. Here is something about trace,

$$\begin{cases} \mathrm{Tr}A = \mathrm{Tr}[a_{ij}]_{i,j=1,2,\dots n} = \sum_{i=1}^{n} a_{ii} \\ A \geq 0 \text{A is a positive semidefinite matrix,} \mathrm{Tr}A = 1, \\ \text{A represents quantum state} \end{cases} \quad (3)$$

First, from $U \cdot H \cdot U^{*}=\begin{pmatrix} d_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & d_n \end{pmatrix}$, we have $H=U^{*}\begin{pmatrix} d_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & d_n \end{pmatrix}U$, which defines the Hermitian matrix. Let us set $A = UDU^{*}$, $B = VFV^{*}$, F as a diagonal matrix, $F=\begin{pmatrix} f_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & f_n \end{pmatrix}$ and $f_j \geq 0$. So we have $A \otimes B = (UDU^{*}) \otimes (VFV^{*}) = (U \otimes V)(D \otimes F)(U^{*} \otimes V^{*})$. For the Kronecker product of two unitary matrices, If $UU^{*} = I_m$, $VV^{*}= I_n$, we have U and V as unitary matrices.

Step 1, $A, B \geq 0$, $A \otimes B \geq 0$

Step 2, Suppose $A_1, \dots A_{n-1} \geq 0$, then $A_1 \otimes \dots \otimes A_{n-1} \geq 0$

Step 3, $A_n \geq 0$, $A_1 \otimes \dots \otimes A_{n-1} \otimes A_n = (A_1 \otimes \dots \otimes A_{n-1}) \otimes A_n \geq 0$, by using step 1.

We set $A = UDU^{*}$ and $B = VFV^{*}$, D, and F as diagonal matrices; d_i and f_j are real numbers. Finally, we have if $A \otimes B \geq 0$, then we have $\begin{cases} A \geq 0, B \geq 0 \\ A \leq 0, B \leq 0 \end{cases}$.

2.4 Injection, bijection, surjection and linear map

We show the transpose of a matrix, the one-to-one correspondence between the transposed matrix and the original matrix. Forming a one-to-one correspondence between these two matrices and such a relationship is also called bijection in set theory.

Lemma 2.4.1. Suppose $x \in M_n, x = \begin{bmatrix} m_{1,1} & \cdots & m_{1,n} \\ \vdots & \ddots & \vdots \\ & & \\ m_{n,1} & \cdots & m_{n,n} \end{bmatrix}, m_{j,j} \in C$, then we have $Tr: M_n \to C = \{a + bi \mid a, b \in R\}$ is surjective.

Proof. We set $x=\begin{bmatrix} y & 0 & \cdots & 0 \\ & & & \\ 0 & 0 & 0 & \vdots \\ \vdots & \vdots & \ddots & 0 \\ & & & \\ 0 & \cdots & \cdots & 0 \end{bmatrix}$, such that $Tr\, x = y$, we obtain f is surjective.

Another question is whether $Tr: M_n \to C = \{a + bi \mid a, b \in R\}$ is injective.

Proof. If we have$\mathrm{Tr} z = 0 + \cdots + 0 + y = y$, so $Tr\, x = Tr\, z$, but $x \neq z$. If $\forall y \in C, \exists x, z \in M_n$, we have $\mathrm{Tr}\, x = \mathrm{Tr}\, z$, but $x \neq z$. Then, we obtain the Trace function, which is not injective.

Subsequently, we show something about mappings in set theory. For a function like this:

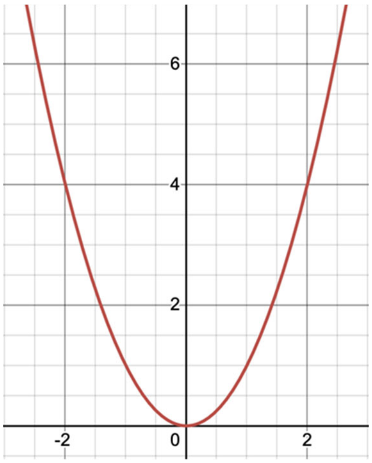

Fig. 1 Graph of $y = x^2$

f: $x \rightarrow x^2$, which means $R \rightarrow R^+ \cup \{0\}$, and from the graph, *f* is not bijective for the function $y = 2^x$.

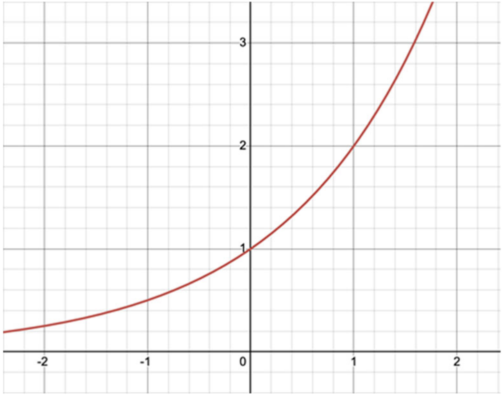

Fig. 2 Graph of $y = 2^x$

f : x → 2^x, which means $R \longleftrightarrow R^+ \subset R$, this is also one-to-one correspondence. $\forall y = 2^x$, we have $x = \log_2 y$, and $y > 0$. Besides, this is a linear map for this operation $(A + B)^T = A^T + B^T$; this is a linear map.

3. Result

3.1 Bipartite Hermitian matrix and bipartite positive semidefinite matrix

We know that:

$$H = H^* \text{ is equivalent to } H \text{ is Hermitian, and } H \in M_n.$$

Definition 3.1.1. $H_1 \in \mathcal{M}_m \otimes \mathcal{M}_n = \mathcal{B}(H_A \otimes H_B)$.

We know that the blocks H_1, $K_{1,1}$ . . . $K_{1,m}$ form the first block row, and the blocks $K_{1,1}$ . . . $K_{m,1}$ form the first block column. We define the reduced Hermitian matrices of systems A and B as follows,

$$(H_1)_A = \begin{bmatrix} TrK_{1,1} & \cdots & TrK_{1,m} \\ \vdots & \ddots & \vdots \\ TrK_{m,1} & \cdots & TrK_{m,m} \end{bmatrix}, (H_1)_B = \sum_{j=1}^{m} K_{j,j}, \tag{4}$$

Claim 3.1.2. Suppose the matrix H_1 is Hermitian (resp. positive semidefinite). Then, the two matrices $(H_1)_A$ and $(H_1)_B$ are both Hermitian (resp. positive semidefinite).

3.2 Two-qubit case

We have $H_1 = \begin{bmatrix} X_{1,1} & \cdots & X_{1,m} \\ \vdots & \ddots & \vdots \\ X_{m,1} & \cdots & X_{m,m} \end{bmatrix}$, and $H_1 \in \mathcal{M}_{mn}^h \xrightarrow{\mathrm{Tr}_B} (H_1)_A \in \mathcal{M}_m^h \xrightarrow{\mathrm{Tr}_B^{-1}} K \overset{?}{=} H_1 \in \mathcal{M}_{mn}^h$, where m, n > 1, and m, n ∈ N /{1}, K may not equal to H1, for example, we suppose

$H_1=\begin{bmatrix}2&1&2&3\\1&3&3&4\\2&3&3&2\\3&4&2&5\end{bmatrix}$, generally, $K=\begin{bmatrix}2+y&a&2+p&c\\\bar{a}&3\text{-}y&d&4\text{-}p\\2+\bar{p}&\bar{d}&3+w&b\\\bar{c}&4\text{-}\bar{p}&\bar{b}&5\text{-}w\end{bmatrix}=K^*$, where a, b, p, c, d ∈ C, and y, w ∈ R. One can show that K equals H1 if and only if w = y = p = 0, c = d = 3, a = 1 and b = 2. Otherwise, K is not equal to H₁. Then we have $(H_1)_A=\begin{bmatrix}5&6\\6&8\end{bmatrix}$ and $(H_1)_B=\begin{bmatrix}5+y+w&a+b\\\bar{a}+\bar{b}&8\text{-}y\text{-}w\end{bmatrix}$

Lemma 3.2.1. We have Tr A_1 = Tr B_1 = 1, then exist M ∈ $M_m \otimes M_n$, such that $M_A = A_1$ and $M_B = B_1$, and one example is $M = A_1 \otimes B_1$.

Definition 3.2.2. The definition of linear combination is that if $X \in C^m=\text{span}\{e_1,..., e_m\}$, then $X=\sum_{j=1}^{m} x_j e_j, x_j \in C$.

We can define that $Tr = Tr_A \otimes Tr_B: M_{AB} \rightarrow C$, and $Tr_A\, M_{AB} = M_B$, and $Tr_B\, M_{AB} = M_A$, and $Tr_A: M_m \otimes M_n \rightarrow M_n$, and $Tr_B: M_m \otimes M_n \rightarrow M_m$.

Lemma 3.2.3. (i) If we have $A_1 \in \mathcal{M}_m^+, B_1 \in \mathcal{M}_n^+$, the condition Tr A_1 = Tr B_1 is sufficient and necessary for the existence of $\rho_{AB} \in (\mathcal{M}_m \otimes \mathcal{M}_n)^+$, such that $\rho_A = A_1$ and $\rho_B = B_1$.

(ii) If we have $A_1 \in \mathcal{M}_m^h, B_1 \in \mathcal{M}_n^h$, the condition Tr A_1 = Tr B_1 is sufficient and necessary for the existence of ρ_{AB}, $\rho_{AB} \in (\mathcal{M}_m \otimes \mathcal{M}_n)^h$, such that $\rho_A = A_1$ and $\rho_B = B_1$.

(iii) Suppose $A_1 \in \mathcal{M}_m^h, B_1 \in \mathcal{M}_n^h$, and Tr A_1 = Tr B_1. Then, there exists $\rho_{AB} \in (\mathcal{M}_m \otimes \mathcal{M}_n)^h$, such that $\rho_A = A_1$ and $\rho_B = B_1$. If $A_1 = \begin{bmatrix}a_1&0\\0&a_2\end{bmatrix}$ and $B_1 = \begin{bmatrix}b_1&0\\0&b_2\end{bmatrix}$, we have $a_1 + a_2 = b_1 + b_2$ because of Tr A_1 = Tr B_1. Then, the general expression of ρ_{AB} is $K_1=\begin{bmatrix}x&d&c&f\\\bar{d}&a_1\text{-}x&g&\text{-}c\\\bar{c}&\bar{g}&b_1\text{-}x&\text{-}d\\\bar{f}&\text{-}\bar{c}&\text{-}\bar{d}&a_2\text{-}b_1+x\end{bmatrix}$, x, a_1, a_2, b_1 ∈ R and d, c, f, g ∈ C.

Proof. (i) If $\rho_{AB} = A_1 \otimes B_1$, then $Tr_B\rho_{AB}=(TrB_1)\cdot A_1=\rho_A=A_1$, and we need Tr B_1 = 1, but the lemma doesn't mention that, so it's not true. We know that $\rho_A=Tr_B\rho_{AB}=A_1$and $\rho_B=Tr_A\rho_{AB}=B_1$, and we have $Tr\rho_A=Tr_A\rho_A=(TrA_1 \otimes TrB_1)\rho_{AB}=Tr\rho_{AB}$, and $Tr\rho_B=Tr_B\rho_B=(TrA_1 \otimes TrB_1)\rho_{AB}=Tr\rho_{AB}$, then we have Tr A_1 = Tr B_1

There are two cases: the first one is that If Tr A_1 = Tr $B_1 \neq 0$, and the second one is that if Tr A_1 = Tr B_1 = 0.

If Tr A_1 = Tr $B_1 \neq 0$, then we have $\rho_{AB} = \frac{A_1 \otimes B_1}{TrA_1}$, such that:

$$\rho_A = Tr_B\rho_{AB} = \sum_{j=1}^{n} (I_m \otimes e_j^T) \cdot \rho_{AB} \cdot (I_m \otimes e_j)$$

$$= \sum_{j=1}^{n} (I_m \otimes e_j^T) \cdot \frac{A_1 \otimes B_1}{TrA_1} \cdot (I_m \otimes e_j)$$

$$= \sum_{j=1}^{n} \frac{A_1 \otimes (e_j^T B_1 e_j)}{TrA_1} = \frac{A_1 \otimes TrB_1}{TrA_1} = \frac{A_1 \cdot TrB_1}{TrA_1} = A_1.$$

$$\rho_B = Tr_A\rho_{AB} = \sum_{i=1}^{m} (e_i^T \otimes I_n) \cdot \rho_{AB} \cdot (e_i \otimes I_n)$$

$$= \sum_{i=1}^{m} (e_i^T \otimes I_n) \cdot \frac{A_1 \otimes B_1}{TrA_1} \cdot (e_i \otimes I_n)$$

$$= \sum_{i=1}^{m} \frac{(e_i^T A_1 e_i) \otimes B_1}{TrA_1} = \frac{TrA_1 \otimes B_1}{TrA_1} = \frac{TrA_1 \cdot B_1}{TrA_1} = B_1.$$

If Tr A_1 = Tr B_1 = 0, we set $A_2 = A_1 + \frac{1}{m} I_m$, and $B_2 = B_1 + \frac{1}{n} I_n$, then we have Tr$A_2$ = TrB_2 = 1.

Then, we have:

$$\rho_{AB} = A_2 \otimes B_2 - \frac{1}{mn} I_{mn} = (A_1 + \frac{1}{m} I_m) \otimes (B_1 + \frac{1}{n} I_n) - \frac{1}{mn} I_{mn}$$

$$= A_1 \otimes B_1 + \frac{1}{n} A_1 \otimes I_n + \frac{1}{m} I_m \otimes B_1 + \frac{1}{mn} I_m \otimes I_n - \frac{1}{mn} I_{mn}$$

$$= A_1 \otimes B_1 + \frac{1}{n} A_1 \otimes I_n + \frac{1}{m} I_m \otimes B_1.$$

$$\rho_A = Tr_B\rho_{AB} = Tr_B(A_1 \otimes B_1 + \frac{1}{n} A_1 \otimes I_n + \frac{1}{m} I_m \otimes B_1) = A_1 \cdot TrB_1 + \frac{1}{n} A_1 \cdot TrI_n + \frac{1}{m} I_m \cdot TrB_1 = \frac{1}{n} A_1 \cdot n = A_1.$$

$$\rho_B = Tr_A\rho_{AB} = Tr_A(A_1 \otimes B_1 + \frac{1}{n} A_1 \otimes I_n + \frac{1}{m} I_m \otimes B_1)$$

$$= TrA_1 \cdot B_1 + \frac{1}{n} TrA_1 \cdot I_n + \frac{1}{m} TrI_m \cdot B_1$$

$$= \frac{1}{m} \cdot m \cdot B_1 = B_1.$$

In conclusion, we have $\rho_A = A_2 - \frac{1}{m} I_m = A_1, \rho_B = B_2 - \frac{1}{n} I_n = B_1$, so the condition Tr$A_1$ = Tr B_1 is sufficient and necessary for ρ_{AB}.

(ii) If $A_1 = \begin{bmatrix} a_1 & 0 \\ 0 & a_2 \end{bmatrix}$, $B_1 = \begin{bmatrix} b_1 & 0 \\ 0 & b_2 \end{bmatrix}$, and $a_j \in R$, $b_j \in R$, also we know that $a_1 + a_2 = b_1 + b_2$. Then, we find $K_1 = \begin{bmatrix} x & d & c & f \\ \bar{d} & a_1 - x & g & -c \\ \bar{c} & \bar{g} & y & -d \\ \bar{f} & -\bar{c} & -\bar{d} & a_2 - y \end{bmatrix} \in \mathcal{M}_4^h$, such that $Tr_B K_1 = A_1$ and $Tr_A K_1 = B_1$, there $\rho_{AB} = K_1$. General, if we have order-2 Hermitian matrices A_2 and B_2 and unitary matrices U and V, such that $UA_2U^* = A_1$, and $VB_2V^* = B_1$. We have $Tr_A K_2 = B_2$, then we have:

$$Tr_A[e_{ij} \otimes c_{ij}] = B_2,$$

$$Tr_A[e_{ij} \otimes c_{ij}]$$

$$= (Tr_A e_{ij}) \otimes c_{ij}$$

$$= (Tr_A(Ue_{ij}U^*)) \otimes c_{ij}$$

$$= Tr_A[(Ue_{ij}U^*) \otimes c_{ij}]$$

$$= Tr_A[\sum_{i,j=1}^{2} (Ue_{ij}U^*) \otimes Vc_{ij}V^*] = VB_2V^*,$$

$$\mathrm{Tr_A}[\sum_{i,j=1}^{2} (\mathrm{Ue_{ij}U^*}) \otimes \mathrm{Vc_{ij}V^*}] = \mathrm{Tr_A}[(\mathrm{U} \otimes \mathrm{V})(\sum_{i,j=1}^{2} \mathrm{e_{ij}} \otimes \mathrm{c_{ij}})(\mathrm{U^*} \otimes \mathrm{V^*})]. \tag{5}$$

Then we have $\mathrm{Tr_A}[(\mathrm{U}\otimes\mathrm{V})\cdot\mathrm{K_2}\cdot(\mathrm{U}\otimes\mathrm{V})^*]=\mathrm{VB_2V^*}=\mathrm{B_1}$. Also $\mathrm{Tr}_B K_2 = A_2$, then we have:

$$Tr_B[e_{ij} \otimes c_{ij}] = A_2,$$

$$Tr_B[e_{ij} \otimes c_{ij}]$$

$$= (Tr_B e_{ij}) \otimes c_{ij}$$

$$= (Tr_B(Ue_{ij}U^*)) \otimes c_{ij}$$

$$= Tr_B[(Ue_{ij}U^*) \otimes c_{ij}]$$

$$= Tr_B[\sum_{i,j=1}^{2} (Ue_{ij}U^*) \otimes Vc_{ij}V^*] = UA_2U^*,$$

And we have:

$$\mathrm{Tr_B}[\sum_{i,j=1}^{2} (\mathrm{Ue_{ij}U^*}) \otimes \mathrm{Vc_{ij}V^*}] = \mathrm{Tr_B}[(\mathrm{U}\otimes\mathrm{V})\cdot\mathrm{K_2}\cdot(\mathrm{U}\otimes\mathrm{V})^*]. \tag{6}$$

Then, we have $\mathrm{Tr_B}[(\mathrm{U}\otimes\mathrm{V})\cdot\mathrm{K_2}\cdot(\mathrm{U}\otimes\mathrm{V})^*]=\mathrm{UA_2U^*}=\mathrm{A_1}$, then, we obtain $K_1 = (U \otimes V)K_2(U \otimes V)^*$ and $\mathrm{K_2}=(\mathrm{U}\otimes\mathrm{V})^*\mathrm{K_1}(\mathrm{U}\otimes\mathrm{V})$.

Theorem 3.2.4. Suppose $\mathrm{A_1}=\begin{bmatrix} \mathrm{a_1} & 0 \\ 0 & \mathrm{a_2} \end{bmatrix}$, $\mathrm{a_i} \geq 0$ and $\mathrm{B_1}=\begin{bmatrix} \mathrm{b_1} & 0 \\ 0 & \mathrm{b_2} \end{bmatrix}$, $\mathrm{b_j} \geq 0$, and $\mathrm{a_1}+\mathrm{a_2}=\mathrm{b_1}+\mathrm{b_2}$. There exists $\rho_{AB} \in (\mathcal{M}_m \otimes \mathcal{M}_n)^h$, such that $\rho_A = A_1$ and $\rho_B = B_1$. If ρ_{AB} is positive semidefinite, then the general expression of ρ_{AB} is $\mathrm{K_1}=\begin{bmatrix} \mathrm{x} & \mathrm{d} & \mathrm{c} & \mathrm{f} \\ \bar{\mathrm{d}} & \mathrm{a_1}\text{-}\mathrm{x} & \mathrm{g} & \text{-}\mathrm{c} \\ \bar{\mathrm{c}} & \bar{\mathrm{g}} & \mathrm{b_1}\text{-}\mathrm{x} & \text{-}\mathrm{d} \\ \bar{f} & \text{-}\bar{\mathrm{c}} & \text{-}\bar{\mathrm{d}} & \mathrm{a_2}\text{-}\mathrm{b_1}\text{+}\mathrm{x} \end{bmatrix}$, $x, a_1, a_2, b_1 \in \mathrm{R}$ *and* $d, c, f, g \in \mathrm{C}$. Up to local unitary equivalence, we can assume that:

$$a_1 \geq b_1 \geq b_2 \geq a_2 \geq 0. \tag{7}$$

By Theorem 2.3.1., if K_1 is positive semidefinite, then we have $x \geq 0$, $a_1 - x \geq 0$, $b_1 - x \geq 0$, $a_2 - b_1 + x \geq 0$,

$$b_1 - a_2 = max\{0, b_1 - a_2\} \leq x \leq min\{a_1, b_1\} = b_1. \tag{8}$$

In the following, by using Theorem 2.3.1., we need to investigate the determinants of the 11 submatrices of the matrix K_1. They are given as follows.

$$det\begin{bmatrix} x & f \\ \bar{f} & a_2 - b_1 + x \end{bmatrix} = x(a_2 - b_1 + x) - f \cdot \bar{f}, \tag{9}$$

$$det\begin{bmatrix} a_1 - x & -c \\ & \\ -\bar{c} & a_2 - b_1 + x \end{bmatrix} = (a_1 - x)(a_2 - b_1 + x) - c \cdot \bar{c}, \tag{10}$$

$$= a_1b_1x - a_1x^2 - b_1x^2 + x^3 - a_1c\bar{c} + dg\bar{c} + cx\bar{c} - b_1d\bar{d} + dx\bar{d} - gx\bar{g} + c\bar{d}\bar{g}, \tag{11}$$

$$= (a_2 - b_1 + x)(b_1x - x^2 - c\bar{c}) + (-dx - f\bar{c})\bar{d} + (-cd - b_1f + fx)f, \tag{12}$$

$$det\begin{bmatrix} a_1 - x & g & -c \\ \bar{g} & b_1 - x & -d \\ -\bar{c} & -\bar{d} & a_2 - b_1 + x \end{bmatrix} = -((b_1c - dg - cx)\bar{c}) + \bar{d}(-a_1d + dx + c\bar{g}) + (a_2 - b_1 + x)(a_1b_1 - a_1x - b_1x + x^2 - gg), \tag{13}$$

$$= -\bar{c}(b_1cx - dgx - cx^2 - c^2\bar{c} - fg\bar{c} + cd\bar{d} + b_1f\bar{d} - fx\bar{d}) \bar{d}(-a_1dx + dx^2 - cd\bar{c} - a_1f\bar{c} + fx\bar{c} + d^2\bar{d} + cx\bar{g} + f\bar{d}\bar{g}), \tag{14}$$

$$\frac{a_1 - \sqrt{(a_1)^2 - 4|d|^2}}{2} \le x \le \frac{a_1 + \sqrt{(a_1)^2 - 4|d|^2}}{2} \tag{15}$$

$$\frac{b_1 - \sqrt{(b_1)^2 - 4|c|^2}}{2} \le x \le \frac{b_1 + \sqrt{(b_1)^2 - 4|c|^2}}{2} \tag{16}$$

$$x \le \frac{(b_1 - a_2) - \sqrt{(a_2 - b_1)^2 + 4|f|^2}}{2} \text{ or} \tag{17}$$

$$x \ge \frac{(b_1 - a_2) + \sqrt{(a_2 - b_1)^2 + 4|f|^2}}{2} \tag{18}$$

$$\frac{1}{2}(a_1 - a_2 + b_1) - \frac{1}{2}\sqrt{a_1^2 + 2a_1a_2 + a_2^2 - 2a_1b_1 - 2a_2b_1 + b_1^2 - 4|c|^2} \le x \le \frac{1}{2}(a_1 - a_2 + b_1) + \frac{1}{2}\sqrt{a_1^2 + 2a_1a_2 + a_2^2 - 2a_1b_1 - 2a_2b_1 + b_1^2 - 4|c|^2} \tag{19}$$

$$\frac{2b_1 - a_2 - \sqrt{a_2^2 - 4|d|^2}}{2} \le x \le \frac{2b_1 - a_2 + \sqrt{a_2^2 - 4|d|^2}}{2} \tag{20}$$

We set $a_2 = 3$, $d = 1$, $c = 2$, $f = 1$, $g = 2$, and a_1, b_1 as parameters, then according to 6 inequalities of x, from (20) to (25), we have a cube that integrates each of the solid regions represented by the six inequalities, and six separate regions to represent the region of x in each of the six inequalities.

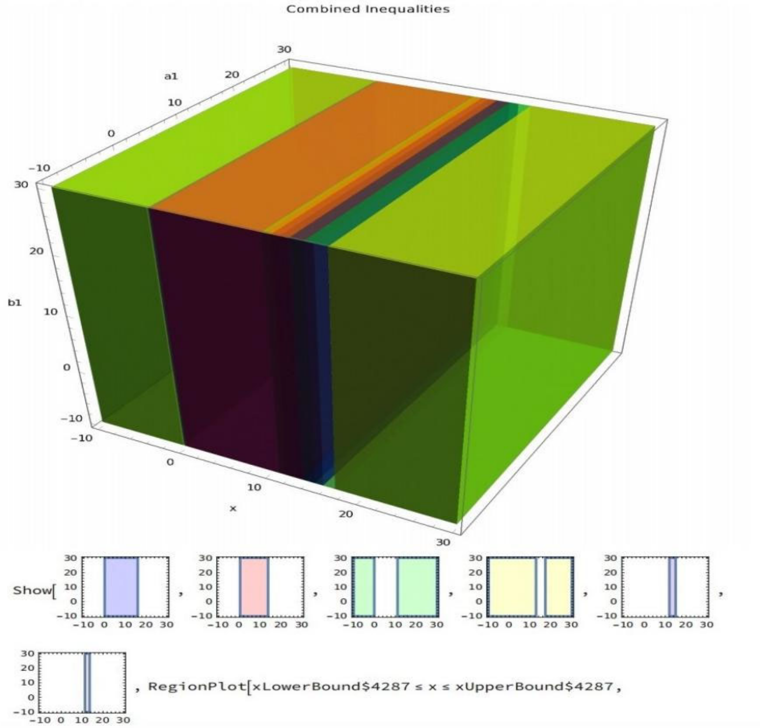

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Fig.3 The regions which represent the inequalities of x, $a_1 = 16$ and $b_1 = 14$

3.3 Three-qubit case

We can see the 8 × 8 Hermitian matrix $M_{ABC} = [m_{ij}]_{i,j=1,\ldots,8}$, $m_{ij} = \overline{m_{ji}}$, $M_{ABC} = M^*_{ABC} = \begin{bmatrix} N_{11} & N_{12} \\ N_{21} & N_{22} \end{bmatrix} = \begin{bmatrix} P_{11} & P_{12} & P_{13} & P_{14} \\ P_{21} & P_{22} & P_{23} & P_{24} \\ P_{31} & P_{32} & P_{33} & P_{34} \\ P_{41} & P_{42} & P_{43} & P_{44} \end{bmatrix}$, Here, N_{ij} are 4 × 4 matrices and P_{ij} are 2 × 2 matrices. Then we have $N_{BC} = N_{11} + N_{22}$, and

$$N_{AC} = \begin{bmatrix} P_{11} + P_{22} & P_{13} + P_{24} \\ P_{31} + P_{42} & P_{33} + P_{44} \end{bmatrix},$$

Suppose N_{AB}, N_{BC}, and N_{AC} come from the Hermitian matrix N_{ABC}. We have:

$$\mathcal{N}_{ABC} = \begin{bmatrix} P_{11} + Q_{11} & P_{12} + Q_{12} & P_{13} + Q_{13} & P_{14} + Q_{14} \\ P_{21} + Q_{21} & P_{22} + Q_{22} & P_{23} + Q_{23} & P_{24} + Q_{24} \\ P_{31} + Q_{31} & P_{32} + Q_{32} & P_{33} + Q_{33} & P_{34} + Q_{34} \\ P_{41} + Q_{41} & P_{42} + Q_{42} & P_{43} + Q_{43} & P_{44} + Q_{44} \end{bmatrix}.$$

Here, P_{ij} and Q_{ij} are 2 × 2 matirces, $P_{ij} = P^*_{ji}$ and $Q_{ij} = Q^*_{ji}$, then

$$\mathcal{N}_{BC} = \begin{bmatrix} (P_{11} + Q_{11}) + (P_{33} + Q_{33}) & (P_{12} + Q_{12}) + (P_{34} + Q_{34}) \\ (P_{21} + Q_{21}) + (P_{43} + Q_{43}) & (P_{22} + Q_{22}) + (P_{44} + Q_{44}) \end{bmatrix},$$

$$\mathcal{N}_{AB} = \begin{bmatrix} \mathrm{Tr}(P_{11} + Q_{11}) & \mathrm{Tr}(P_{12} + Q_{12}) & \mathrm{Tr}(P_{13} + Q_{13}) & \mathrm{Tr}(P_{14} + Q_{14}) \\ \mathrm{Tr}(P_{21} + Q_{21}) & \mathrm{Tr}(P_{22} + Q_{22}) & \mathrm{Tr}(P_{23} + Q_{23}) & \mathrm{Tr}(P_{24} + Q_{24}) \\ \mathrm{Tr}(P_{31} + Q_{31}) & \mathrm{Tr}(P_{32} + Q_{32}) & \mathrm{Tr}(P_{33} + Q_{33}) & \mathrm{Tr}(P_{34} + Q_{34}) \\ \mathrm{Tr}(P_{41} + Q_{41}) & \mathrm{Tr}(P_{42} + Q_{42}) & \mathrm{Tr}(P_{43} + Q_{43}) & \mathrm{Tr}(P_{44} + Q_{44}) \end{bmatrix},$$

$$\mathcal{N}_{AC} = \begin{bmatrix} (P_{11} + Q_{11}) + (P_{22} + Q_{22}) & (P_{13} + Q_{13}) + (P_{24} + Q_{24}) \\ (P_{31} + Q_{31}) + (P_{42} + Q_{42}) & (P_{33} + Q_{33}) + (P_{44} + Q_{44}) \end{bmatrix}.$$

Then we have $Q_{22} = Q_{33} = -Q_{11} = -Q_{44}$, $Q_{12} = -Q_{34}$, $Q_{21} = -Q_{43}$, $Q_{13} = -Q_{24}$, $Q_{31} = -Q_{42}$, and the traces of all Q_{ij} are 0. Then we have

$$\mathcal{N}_{ABC} = \begin{bmatrix} P_{11}+Q_{11} & P_{12}+Q_{12} & P_{13}+Q_{13} & P_{14}+Q_{14} \\ P_{21}+Q_{21} & P_{22}+Q_{22} & P_{23}+Q_{23} & P_{24}+Q_{24} \\ P_{31}+Q_{31} & P_{32}+Q_{32} & P_{33}+Q_{33} & P_{34}+Q_{34} \\ P_{41}+Q_{41} & P_{42}+Q_{42} & P_{43}+Q_{43} & P_{44}+Q_{44} \end{bmatrix}$$
$$= \begin{bmatrix} P_{11}+Q_{11} & P_{12}+Q_{12} & P_{13}+Q_{13} & P_{14}+Q_{14} \\ P_{21}+Q_{21} & P_{22}+Q_{22} & P_{23}+Q_{23} & P_{24}-Q_{13} \\ P_{31}+Q_{31} & P_{32}+Q_{32} & P_{33}+Q_{22} & P_{34}-Q_{12} \\ P_{41}+Q_{41} & P_{42}-Q_{31} & P_{43}-Q_{21} & P_{44}+Q_{11} \end{bmatrix}$$

4. Conclusion

We have investigated the maps from a bipartite Hermitian matrix H to two single-system reduced Hermitian matrices H_A and H_B, as well as the inverse problem. We explicitly obtained the expressions of the abovementioned matrices. We further studied the subcase of positive semidefinite H such that H_A and H_B are also positive semidefinite. The subcase has been dealt with regarding 15 determinants of submatrices from H. We characterized the parameters in these matrices to determine the positive semidefiniteness of H. Then, we extend our results to three-qubit matrices. Our study helps us understand the mathematical structure of multipartite system density operators. They are important notions from quantum physics and information theory, so our results may be applied to more problems.

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