

Separability of three qubit Greenberger-Horne-Zeilinger diagonal states

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Seung-Hyeok Kye (Seoul National University)
a joint work with Kyung Hoon Han

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1. Greenberger-Horne-Zeilinger diagonal states

A state on the Hilbert space $\mathcal{H} = \mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2} \otimes \dots \otimes \mathbb{C}^{d_n}$ is said to be *(fully) separable* if it is the convex combination

$$\varrho := \sum_{i \in I} p_i |z_i\rangle\langle z_i|$$

of *pure product states* $|z_i\rangle\langle z_i|$ onto *product vectors* $|z_i\rangle$:

$$|z_i\rangle = |x_{1i}\rangle \otimes |x_{2i}\rangle \otimes \dots \otimes |x_{ni}\rangle \in \mathbb{C}^{d_1} \otimes \mathbb{C}^{d_2} \otimes \dots \otimes \mathbb{C}^{d_n}, \quad i \in I.$$

Therefore, ϱ is a $d \times d$ density matrix, with the dimension $d = \prod_{i=1}^n d_i$ of the Hilbert space \mathcal{H} . The set consisting of all separable states is a convex set whose extreme points are pure product states.

A state which is not separable is call *entangled*.

To get entanglement, we begin with **non-product** vector, say

$$\begin{aligned} |\xi\rangle &= |00\rangle + |11\rangle \in \mathbb{C}^2 \otimes \mathbb{C}^2 \\ &= |0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle \\ &= (1, 0)^t \otimes (1, 0)^t + (0, 1)^t \otimes (0, 1)^t \in \mathbb{C}^2 \otimes \mathbb{C}^2 \\ &= (1, 0, 0, 1)^t \in \mathbb{C}^4 \end{aligned}$$

and take pure state

$$|\xi\rangle\langle\xi| = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} (1, 0, 0, 1) = \begin{pmatrix} 1 & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & 1 \end{pmatrix}.$$

The **partial transpose** (= block-wise transpose):

$$\begin{pmatrix} 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot \\ \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 \end{pmatrix}.$$

is not positive (=positive semi-definite).

- In general, $\rho \in M_m \otimes M_n$ is separable \implies PPT.
Choi (1982), Peres (1996)
- The converse holds if and only if $(m, n) = (2, 2), (2, 3)$ or $(3, 2)$.
Størmer (1963), Woronowicz (1976), Choi (1982), Horodecki's (1996)

It is extremely difficult in general to distinguish entanglement from separability.

Actually, it is known to be an *NP*-hard problem [Gurvits (2004)].

The three qubit **GHZ state basis** consists of eight vectors in $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$ given by

$$|\xi_{ijk}\rangle = \frac{1}{\sqrt{2}} (|i\rangle \otimes |j\rangle \otimes |k\rangle + (-1)^i |\bar{i}\rangle \otimes |\bar{j}\rangle \otimes |\bar{k}\rangle), \quad i + \bar{i} = 1 \pmod{2}$$

where the index ijk runs for $i, j, k \in \{0, 1\}$. We may write down as follows:

$$|000\rangle + |111\rangle = (1, 0, 0, 0, 0, 0, 0, 1)$$

$$|001\rangle + |110\rangle = (0, 1, 0, 0, 0, 0, 1, 0)$$

$$|010\rangle + |101\rangle = (0, 0, 1, 0, 0, 1, 0, 0)$$

$$|011\rangle + |100\rangle = (0, 0, 0, 1, 1, 0, 0, 0)$$

$$|100\rangle - |011\rangle = (0, 0, 0, -1, 1, 0, 0, 0)$$

$$|101\rangle - |010\rangle = (0, 0, -1, 0, 0, 1, 0, 0)$$

$$|110\rangle - |001\rangle = (0, -1, 0, 0, 0, 0, 1, 0)$$

$$|111\rangle - |000\rangle = (-1, 0, 0, 0, 0, 0, 0, 1)$$

We endow the indices with the lexicographic order to get eight vectors $\xi_1, \xi_2, \dots, \xi_8$. A **GHZ diagonal** state is of the form

$$\rho = \sum_{i=1}^8 p_i |\xi_i\rangle \langle \xi_i|$$

for nonnegative p_i 's with $\sum_{i=1}^8 p_i = 1$.

So, ρ is X-shaped;

$$X(a, b, c) := \begin{pmatrix} a_1 & & & & & & & c_1 \\ & a_2 & & & & & & c_2 \\ & & a_3 & & & & & c_3 \\ & & & a_4 & c_4 & & & \\ & & & \bar{c}_4 & b_4 & & & \\ & & & & & & & \\ & & & & & & b_3 & \\ & & & \bar{c}_3 & & & & \\ & & & & & & & \\ & \bar{c}_2 & & & & & & b_2 \\ \bar{c}_1 & & & & & & & b_1 \end{pmatrix}.$$

$\rho = \frac{1}{2}X(a, b, c)$ with

$$\begin{aligned} a = b &= (p_1 + p_8, p_2 + p_7, p_3 + p_6, p_4 + p_5), \\ c &= (p_1 - p_8, p_2 - p_7, p_3 - p_6, p_4 - p_5). \end{aligned}$$

Conversely, every X -shaped state $X(a, b, c)$ can be realized as a GHZ diagonal state whenever $a = b$ and $c \in \mathbb{R}^4$.

Goal: Characterize separability of $X(a, a, c)$ when $a_i \geq 0$ and c_i is real.

In three qubit case, there are three kinds of partial transpose. Separability implies positivity of these partial transposes.

Describe GHZ diagonal states, using **Pauli matrices**

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

as

$$\begin{aligned} X(a, a, c) = & \frac{1}{8} (I \otimes I \otimes I + \lambda_2 Z \otimes Z \otimes I + \lambda_3 Z \otimes I \otimes Z + \lambda_4 I \otimes Z \otimes Z \\ & + \lambda_5 X \otimes X \otimes X + \lambda_6 Y \otimes Y \otimes X \\ & + \lambda_7 Y \otimes X \otimes Y + \lambda_8 X \otimes Y \otimes Y), \end{aligned}$$

with the coefficients

$$\lambda_2 = 2(+a_1 + a_2 - a_3 - a_4),$$

$$\lambda_3 = 2(+a_1 - a_2 + a_3 - a_4),$$

$$\lambda_5 = 2(+c_1 + c_2 + c_3 + c_4),$$

$$\lambda_7 = 2(-c_1 + c_2 - c_3 + c_4),$$

$$\lambda_4 = 2(+a_1 - a_2 - a_3 + a_4),$$

$$\lambda_6 = 2(-c_1 - c_2 + c_3 + c_4),$$

$$\lambda_8 = 2(-c_1 + c_2 + c_3 - c_4).$$

- A. Kay (2011): A GHZ diagonal state is separable if and only if it is of PPT, whenever $\prod_{i=5}^8 \lambda_i < 0$.
- O. Gühne (2011): the inequality

$$8 \min\{a_1, a_2, a_3, a_4\} \geq \sqrt{\frac{(\lambda_5\lambda_6 + \lambda_7\lambda_8)(\lambda_5\lambda_7 + \lambda_6\lambda_8)(\lambda_5\lambda_8 + \lambda_6\lambda_7)}{\lambda_5\lambda_6\lambda_7\lambda_8}}$$

is a sufficient criterion for the separability of GHZ diagonal states, when $\prod_{i=5}^8 \lambda_i > 0$.

Gühne also gave a necessary condition: Define

$$\mathcal{L}(\varrho, z) := \operatorname{Re}(z_1 c_1 + z_2 c_2 + z_3 c_3 + z_4 \bar{c}_4),$$

$$\mathcal{F}(z) := \operatorname{Re}(z_1) \cos(\alpha + \beta + \gamma) - \operatorname{Im}(z_1) \sin(\alpha + \beta + \gamma) + \operatorname{Re}(z_2) \cos(\alpha) - \\ + \operatorname{Re}(z_3) \cos(\beta) - \operatorname{Im}(z_3) \sin(\beta) + \operatorname{Re}(z_4) \cos(\gamma) - \operatorname{Im}(z_4) \sin(\gamma),$$

$$C(z) := \sup_{\alpha, \beta, \gamma} |\mathcal{F}(z)|$$

and showed that that if $\varrho = X(a, b, c)$ is separable then the inequality

$$\mathcal{L}(\varrho, z) \leq C(z) \Delta_\varrho$$

holds for every $z \in \mathbb{C}^4$, where the number Δ_ϱ is given by

$$\Delta_\varrho = \min\{\sqrt{a_i b_i} \ (i = 1, 2, 3, 4), \sqrt[4]{a_1 b_2 b_3 a_4}, \sqrt[4]{b_1 a_2 a_3 b_4}\}$$

which is determined by the diagonal entries of $\varrho = X(a, b, c)$.

Note: $\Delta_\varrho = \min\{a_i \ (i = 1, 2, 3, 4)\}$, when ϱ is a GHZ diagonal state.

We show:

- Gühne's necessary condition is also sufficient.
We get the formula of $C(z)$ in terms of variables z_i 's.
- In case $\prod_{i=5}^8 \lambda_i \geq 0$, we find the dichotomy with a condition $[\star]$ in terms of anti-diagonal entries c_i 's:
 - ▷ If $[\star]$ does not hold, then separable = PPT.
 - ▷ If $[\star]$ holds, then Gühne's sufficient condition is also necessary.

Our main tool is to use the duality between tri-tensor product and bi-linear maps.

2. Entanglement witnesses

For a multi-linear map ϕ from $M_{d_1} \times \cdots \times M_{d_{n-1}}$ into M_{d_n} , we associate a matrix $C_\phi \in M_d$ by

$$C_\phi = \sum_{i_1, j_1, \dots, i_{n-1}, j_{n-1}} |i_1\rangle\langle j_1| \otimes \cdots \otimes |i_{n-1}\rangle\langle j_{n-1}| \otimes \phi(|i_1\rangle\langle j_1|, \dots, |i_{n-1}\rangle\langle j_{n-1}|) \\ \in M_{d_1} \otimes \cdots \otimes M_{d_{n-1}} \otimes M_{d_n}$$

The correspondence $\phi \mapsto C_\phi$ is nothing but the [Choi-Jamiołkowski isomorphism](#) for bi-partite case of $n = 2$.

We also define the bilinear pairing between ϱ in $M_{d_1} \otimes \cdots \otimes M_{d_{n-1}} \otimes M_{d_n}$ and a multi-linear map $\phi : M_{d_1} \times \cdots \times M_{d_{n-1}} \rightarrow M_{d_n}$ by

$$\langle \varrho, \phi \rangle = \langle \varrho, C_\phi \rangle := \text{Tr}(C_\phi \varrho^\dagger).$$

Theorem (K, J. Phys. A 48 (2015), 235303)

An n -partite state ϱ is (fully) separable if and only if $\langle \varrho, \phi \rangle \geq 0$ for every positive $(n-1)$ -linear map ϕ .

Here, ϕ is **positive** if

$$x_1 \in M_{d_1}^+, \dots, x_{n-1} \in M_{d_{n-1}}^+ \implies \phi(x_1, \dots, x_{n-1}) \in M_{d_n}^+$$

- M. Horodecki, P. Horodecki and R. Horodecki (1996): $n = 2$,
- M. Eom + K (2000): $n = 2$, to find the dual cone of positive maps.

B. M. Terhal (2000)

A non-positive self-adjoint $d \times d$ matrix W is **entanglement witness** if

- $\langle \varrho, W \rangle \geq 0$ for every separable state ϱ .

Then, we have

- every entangled state ϱ is 'detected' by an entanglement witness W in the sense: $\langle \varrho, W \rangle < 0$.
- every entanglement witness W detects an entangled state.

We have interpreted entanglement witnesses as **separate** or **coordinate-wise** positivity of multi-linear maps, which is the weakest notion of positivity.

Observation: Let ϱ be an X-shaped state. Then, ϱ is separable if and only if $\langle \varrho, W \rangle \geq 0$ for every X-shaped entanglement witness W .

For a given $(s, t) \in \mathbb{R}_+^4 \times \mathbb{R}_+^4$ and $u \in \mathbb{C}^4$, we introduce two numbers:

$$A(s, t) = \inf_{r>0} \left[\sqrt{(s_1 r^{-1} + t_4 r)(s_4 r^{-1} + t_1 r)} + \sqrt{(s_2 r^{-1} + t_3 r)(s_3 r^{-1} + t_2 r)} \right]$$

$$B(u) = \max_{\theta} \left(|u_1 e^{i\theta} + \bar{u}_4| + |u_2 e^{i\theta} + \bar{u}_3| \right).$$

Here, \mathbb{R}_+ denotes $[0, \infty)$. Then we see that a three qubit non-positive self-adjoint matrix $W = X(s, t, u)$ is an entanglement witness if and only if the inequality $A(s, t) \geq B(u)$ holds [Han + K, J. Math. Phys. (2016)].

Theorem

For $z \in \mathbb{C}^4$, we have $C(z) = B(z_1, z_2, z_3, \bar{z}_4)$.

Recall that $C(z)$ was defined as the maximum of a three variable function.

We say that an X-shaped self-adjoint matrix $W = X(s, t, u)$ is **GHZ diagonal** if $s = t$ and $u \in \mathbb{R}$.

Theorem

Let ρ be a GHZ diagonal state. Then, ρ is separable if and only if $\langle \rho, W \rangle \geq 0$ for every GHZ diagonal witness W .

Theorem

Let $\rho = X(a, a, c)$ be a GHZ diagonal state. Then, ρ is separable if and only if the inequality

$$\mathcal{L}(\rho, z) \leq C(z) \Delta_\rho$$

holds for every $z \in \mathbb{R}^4$.

3. Entry-wise characterization

Look for maximum of

$$f(z_1, z_2, z_3, z_4) := \frac{\mathcal{L}(\rho, z)}{C(z)} = \frac{c_1 z_1 + c_2 z_2 + c_3 z_3 + c_4 z_4}{\max_{\theta} (|z_1 e^{i\theta} + z_4| + |z_2 e^{i\theta} + z_3|)}$$

with real z_i 's and c_i 's.

The function f enjoys:

- $f(\alpha z) = f(z)$ for $\alpha > 0$
- $f(-z) = -f(z)$.

We partition the domain of f by $\mathbb{R}^4 \setminus \{0\} = \Omega^+ \sqcup \Omega^-$ with

$$\Omega^+ = \{z \in \mathbb{R}^4 \setminus \{0\} : z_1 z_2 z_3 z_4 \geq 0\}, \quad \Omega^- = \{z \in \mathbb{R}^4 \setminus \{0\} : z_1 z_2 z_3 z_4 < 0\}.$$

We also partition Ω^- by Ω_i^- ($i = 0, 1, 2, 3, 4$)

$$\Omega_i^- = \left\{ z \in \Omega^- : \frac{1}{|z_i|} \geq \sum_{j \neq i} \frac{1}{|z_j|} \right\}, \quad i = 1, 2, 3, 4,$$

$$\Omega_0^- = \Omega^- \setminus \left(\bigsqcup_{i=1}^4 \Omega_i^- \right) = \left\{ z \in \Omega^- : \frac{1}{|z_i|} < \sum_{j \neq i} \frac{1}{|z_j|}, \quad i = 1, 2, 3, 4 \right\}.$$

$z \in \Omega_0^-$ if and only if the reciprocals of entries make a quadrangle.

Theorem

For $z \in \mathbb{R}^4 \setminus \{0\}$, we have

$$C(z) = \begin{cases} |z_1| + |z_2| + |z_3| + |z_4|, & z \in \Omega^+, \\ |z_1| + |z_2| + |z_3| + |z_4| - 2|z_i|, & z \in \Omega_i^- \quad (i = 1, 2, 3, 4), \\ \sqrt{\frac{(z_1 z_2 - z_3 z_4)(z_2 z_4 - z_1 z_3)(z_1 z_4 - z_2 z_3)}{-z_1 z_2 z_3 z_4}}, & z \in \Omega_0^-. \end{cases}$$

Consider only one component of Ω^- , say $z_1 < 0$, $z_i > 0$ ($i = 2, 3, 4$), and restrict the domain of f by $\sum_{i=1}^4 |z_i| = 1$

- The region is the tetrahedron with four extreme points $-E_1, E_2, E_3$ and E_4 .
- Ω_0^- occupies the central part of the tetrahedron touches four extreme points and six edges does not touch four faces
- the boundary between Ω_0^- and Ω_j^- , say Ω_1^- is a two-dimensional surface in the tetrahedron touches the boundary of the face ($=\triangle E_2 E_3 E_4$) opposite to $-E_1$ is far from $-E_1$ and near from the $\triangle E_2 E_3 E_4$

Global behavior of the function f :

- The maximum of f on Ω^+ is $\max |c_i|$.
- No extreme value occurs on the interior of Ω_i^- for $i = 1, 2, 3, 4$.
- f is not differentiable on the boundary between Ω_0^- and Ω_i^- for $i = 1, 2, 3, 4$.
- On this boundary(=two dimensional surface), no extreme value occurs possibly except on a curve where the value of f is $\pm c_i$.

It remains to consider the case the maximum of f occurs on the interior of Ω_0^- .

If an extreme value of f occurs on $s = (s_1, s_2, s_3, s_4) \in \Omega_0^-$, then $t_i = -\frac{1}{s_i}$ is given by

$$t_1 = c_1(+c_1^2 - c_2^2 - c_3^2 - c_4^2) + 2c_2c_3c_4,$$

$$t_2 = c_2(-c_1^2 + c_2^2 - c_3^2 - c_4^2) + 2c_1c_3c_4,$$

$$t_3 = c_3(-c_1^2 - c_2^2 + c_3^2 - c_4^2) + 2c_1c_2c_4,$$

$$t_4 = c_4(-c_1^2 - c_2^2 - c_3^2 + c_4^2) + 2c_1c_2c_3,$$

with the critical value

$$\begin{aligned} f(s_1, s_2, s_3, s_4)^2 &= \frac{(\lambda_5\lambda_6 + \lambda_7\lambda_8)(\lambda_5\lambda_7 + \lambda_6\lambda_8)(\lambda_5\lambda_8 + \lambda_6\lambda_7)}{8^2\lambda_5\lambda_6\lambda_7\lambda_8} \\ &= \frac{(c_1c_2 - c_3c_4)(c_1c_3 - c_2c_4)(c_1c_4 - c_2c_3)}{\lambda_5\lambda_6\lambda_7\lambda_8}, \end{aligned}$$

which appears in the sufficient condition of Gühne.

Using the relation

$$\begin{aligned}(t_2 + t_3)^2 - (t_1 + t_4)^2 &= \lambda_5 \lambda_8 (\lambda_6 \lambda_7)^2, \\ (t_1 - t_4)^2 - (t_2 - t_3)^2 &= \lambda_6 \lambda_7 (\lambda_5 \lambda_8)^2.\end{aligned}$$

One may conclude that the function f has a critical value on Ω_0^- if and only if the inequality $\lambda_5 \lambda_6 \lambda_7 \lambda_8 > 0$ together with the condition $[\star]$:

$$t_1 t_4 \lambda_6 \lambda_7 < 0 \quad \text{and} \quad t_2 t_3 \lambda_5 \lambda_8 > 0 \quad [\star]$$

holds.

Theorem

Let $\rho = X(a, a, c)$ be a GHZ diagonal state with $\lambda_5, \lambda_6, \lambda_7, \lambda_8$ and t_1, t_2, t_3, t_4 given by c_i . Then we have the following:

- (i) if $\lambda_5 \lambda_6 \lambda_7 \lambda_8 \leq 0$, then ρ is separable if and only if it is of PPT,
- (ii) if $\lambda_5 \lambda_6 \lambda_7 \lambda_8 > 0$ and $[\star]$ does not hold, then ρ is separable if and only if it is of PPT,
- (iii) if $\lambda_5 \lambda_6 \lambda_7 \lambda_8 > 0$ and $[\star]$ holds, then ρ is separable if and only if the inequality

$$8 \min\{a_1, a_2, a_3, a_4\} \geq \frac{\sqrt{(\lambda_5 \lambda_6 + \lambda_7 \lambda_8)(\lambda_5 \lambda_7 + \lambda_6 \lambda_8)(\lambda_5 \lambda_8 + \lambda_6 \lambda_7)}}{\sqrt{\lambda_5 \lambda_6 \lambda_7 \lambda_8}}$$

holds.

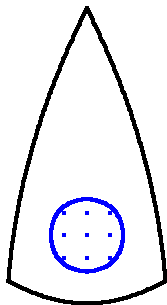
4. Other kinds of separability

In multi-partite case, there are several kinds of separability.

In the tri-partite case, a state $\rho \in M_A \otimes M_B \otimes M_C$ may be considered as a bi-partite states by

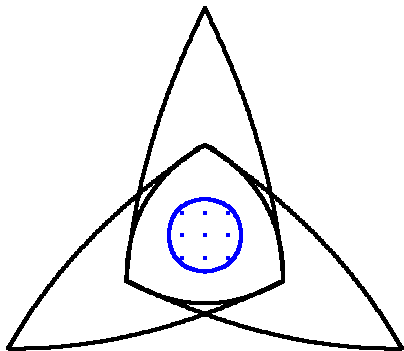
$$\rho \in M_A \otimes M_B \otimes M_C = M_A \otimes (M_B \otimes M_C) = M_A \otimes M_{BC}.$$

Then, we have the notion of A - BC separability as well as full separability.



fully separable

A-BC separable

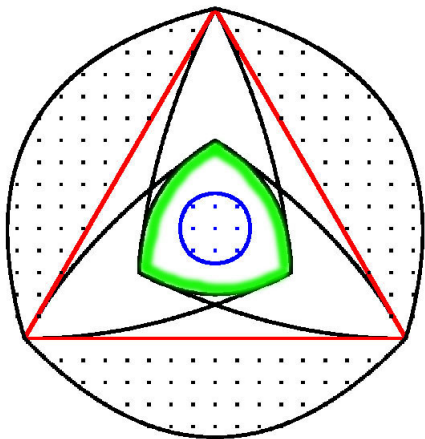


fully separable

$A-BC$ separable

$B-CA$ separable

$C-AB$ separable



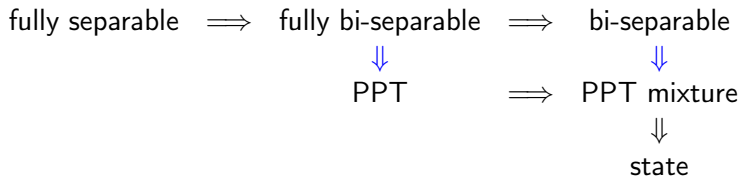
fully separable

fully bi-separable

bi-separable

genuinely entangled

In general, we have the relations:



Blue arrows become equivalence relations for X-states.

Consider the following X-shaped n -qubit cases:

$$\rho = \begin{pmatrix} a_{00\dots 0} & & & & & & & & & & & & & & & & c_{00\dots 0} \\ & \ddots & & & & & & & & & & & & & & & \ddots \\ & & a_{\mathbf{i}} & & & & & & & & & & & & & & c_{\mathbf{i}} \\ & & & \ddots & & & & & & & & & & & & & \ddots \\ & & & & a_{01\dots 1} & & c_{01\dots 1} & & & & & & & & & & \\ & & & & \bar{c}_{01\dots 1} & & b_{01\dots 1} & & & & & & & & & & \\ & & & & & \ddots & & & & & & & & & & & \ddots \\ & & & & & & & & & & & & & & & & \ddots \\ & & & & & & & & & & & & & & & & \ddots \\ \bar{c}_{00\dots 0} & & & & & & & & & & & & & & & & b_{00\dots 0} \end{pmatrix},$$

with \mathbf{i} is an n -multi-index, expressed by an n string of 0,1 beginning with 0.

Theorem (K.-H. Han + K, J. Phys. A 49 (2016), 175303)

For a multi-qubit X -state ρ , we have the following:

- ρ is *fully bi-separable* if and only if it is of *PPT* if and only if $a_i b_i \geq |c_j|^2$ for every i and j
- ρ is *bi-separable* if and only if it is a *PPT-mixture* if and only if $\sum_{j \neq i} \sqrt{a_j b_j} \geq |z_i|$ for each i .

The equivalence between bi-separability and inequality was shown by O. Gühne and M. Seevinck (2010), T. Gao and Y. Hong (2011).

The **arguments** of anti-diagonal entries play **no** role in this cases.

감사합니다.