TRANSFORMATIONS OF ENTANGLED MIXED STATES OF TWO QUBITS

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ABSTRACT

TRANSFORMATIONS OF ENTANGLED MIXED STATES OF TWO QUBITS

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In this thesis, the entangled mixed states of two qubits are considered. In the case where the matrix rank of the corresponding density matrix is 2, such a state can be purified to a pure state of 3 qubits. By utilizing this representation, the classification of such states of two qubits by stochastic local operations assisted by classical communication (SLOCC) is obtained. Also for such states, the optimal ensemble that appears in the computation of the concurrence and entanglement of formation is obtained.

Keywords: Entanglement, Mixed state, SLOCC, Optimal ensemble, Entanglement of formation

ÖZ

İKİ KÜBİTLİ DOLANIK KARIŞIM DURUMLARININ DÖNÜŞÜMLERİ

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Bu tez çalışmasında, iki kübitin dolanık karışım durumları ele alınmıştır. Duruma karşılık gelen yoğunluk matrisinin rankının 2 olması halinde, böyle bir durum 3 kübitin bir saf durumu olarak düşünülebilir. Bu temsil yardımıyla, iki kübitin bu türden durumlarının klasik iletişim yardımıyla stokastik yerel operasyonlara (SLOCC) göre sınıflandırılması elde edilmiştir. Ayrıca, bu tür durumlar için, dolanıklık miktarını hesaplamada kullanılan en uygun topluluk ve 2 kübitin oluşum dolanıklığı elde edilmiştir.

Anahtar Kelimeler: Dolanıklık, Karışım durumu, SLOCC, En uygun topluluk, Oluşum dolanıklığı

To my mother Zahide

and

to my everything, my love, my wife Simge

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CHAPTER 1

INTRODUCTION

Consider the *superposition* postulate of Quantum Mechanics. It leads to the fact that composite quantum systems can be in *entangled* states, i.e., states that are unfactorizable. In the history of quantum physics, the *entanglement* is considered and discussed in depth as the *main reason* of non-locality and quantum correlations. Especially, it started with the criticism of Einstein, Podolsky, and Rosen on the Copenhagen interpretation of quantum mechanics[1] in 1935. In 1964, J. S. Bell has shown that entangled states violate some inequalities, which are called as *Bell inequalities*, which test the non-locality of quantum mechanics which cannot be described classically[2]. After Bell, quantum correlations and non-locality associated with entanglement have been considered as the singlemost important feature of quantum mechanics that distinguishes it from the classical theories[3-9].

On the other hand, entanglement does not appear to be only a subject of discussion or a philosophical issue, but it also appears as an ingredient as a potential resource of the quantum information processing and quantum computation [10-14] in quantum state teleportation [15-26], superdense coding [27,28], and quantum cryptography [29,30]. These works are mainly based on *bipartite pure state* entanglement. The nature, however, also displays multipartite pure state entanglement, about which less is known. In addition to these, *mixed state entanglement* (bipartite or multipartite) occurs naturally as a result of decoherence processes and, mainly for this reason, it is extensively studied. This thesis is concerned some features of the bipartite entangled mixed states. In the following sections, some of the mathematical tools that are used in this thesis are introduced.

1.1 Qubit

In classical information and computation, the fundamental unit of information is *binary digit* (with the abbreviation *bit*), which could be either 0 or 1. In quantum information and computation the fundamental unit is called a *quantum bit* (with the abbreviation *qubit*)[31]. A qubit not only takes the values of either 0 or 1, but also it can take on values which are superpositions of both 0 and 1. In other words, both values are possible for one qubit due to the *superposition principle* in quantum mechanics since qubit is a two-level quantum system [31].

Geometrically, if a bit is a scalar quantity, qubit might be thought as a two-dimensional vectorial quantity which can be decomposed into the orthogonal unit vectors $|0\rangle$ and $|1\rangle$. The vector space of any qubit is a two-dimensional *Hilbert space* denoted by $\mathbb{C}^2$. Using Dirac *bra-ket* notation, after P.A.M. Dirac [32], any qubit is represented by a *ket* which is denoted by a symbol like $|\psi\rangle$ with its dual correspondence *bra* denoted by $\langle\psi|$. Then, an arbitrary qubit in a state $|\psi\rangle$ can be written as a linear combination or superposition of the unit vectors $|0\rangle$ and $|1\rangle$ as follows

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \tag{1.1}$$

where the coefficients α and β are complex numbers. In that case, the *bra* vector is $\langle\psi| = \alpha^*\langle 0| + \beta^*\langle 1|$ where "$*$" represents the complex conjugate. Alternatively, in a one-column matrix (or column vector) notation, mutually orthogonal unit vectors $|0\rangle$ and $|1\rangle$ are taken conventionally as

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{1.2}$$

which form an *orthonormal* basis set for a single qubit. This set $\{|0\rangle, |1\rangle\}$ is called *the computational basis set* in quantum computation. Note that the *bra*'s are then $\langle 0| = \begin{pmatrix} 1 & 0 \end{pmatrix}$ and $\langle 1| = \begin{pmatrix} 0 & 1 \end{pmatrix}$ which are one-row matrices or row vectors. Thus, $|\psi\rangle$ would be written as

$$|\psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \alpha\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta\begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{1.3}$$

Suppose that N qubits are identically prepared in the *pure state* $|\psi\rangle$. If identical measurements on each qubit are made in the computational basis $\{|0\rangle, |1\rangle\}$, then the probability to obtain the outcome 0 is $|\alpha|^2 = \alpha^*\alpha$ and the probability to obtain the outcome 1 is $|\beta|^2 = \beta^*\beta$. These probabilities are called *quantum probabilities*, which are obeying the restriction $|\alpha|^2 + |\beta|^2 = 1$ [33].

1.2 Multiple qubits

When two or more qubits are considered, the tool *tensor product* is used to construct the Hilbert space of the composite system. Let A and B be two qubits with their Hilbert spaces being $\mathcal{H}_1$ and $\mathcal{H}_2$, which are two dimensional. Then the composite system AB for these qubits has the four dimensional Hilbert space $\mathcal{H}_{AB} = \mathcal{H}_1 \otimes \mathcal{H}_2$. Now, let A and B be two local operators (or equivalently matrices) that act separately on each qubit. An operator acting on the whole space $\mathcal{H}_1 \otimes \mathcal{H}_2$ can be constructed by the tensor product as $A \otimes B$. In matrix notation, the tensor product of these operators is calculated by the formula

$$A \otimes B \equiv \begin{pmatrix} A_{11}B & A_{12}B \\ A_{21}B & A_{22}B \end{pmatrix} = \begin{pmatrix} A_{11}B_{11} & A_{11}B_{12} & A_{12}B_{11} & A_{12}B_{12} \\ A_{11}B_{21} & A_{11}B_{22} & A_{12}B_{21} & A_{12}B_{22} \\ A_{21}B_{11} & A_{21}B_{12} & A_{22}B_{11} & A_{22}B_{12} \\ A_{21}B_{21} & A_{21}B_{22} & A_{22}B_{21} & A_{22}B_{22} \end{pmatrix} \tag{1.4}$$

which is called as the *Kronecker product*. Notice that this is a 4×4 matrix.

Therefore, the new four-dimensional computational basis set in $\mathcal{H}_1 \otimes \mathcal{H}_2$ are constructed by the tensor products of the unit vectors $|0\rangle$ and $|1\rangle$

$$|00\rangle_{AB} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}_A \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}_B = \begin{pmatrix} 1\begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ 0\begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix},$$

$$|01\rangle_{AB} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad |10\rangle_{AB} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad |11\rangle_{AB} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}. \tag{1.5}$$

So, an orthonormal basis set in $\mathcal{H}_1 \otimes \mathcal{H}_2$ is

$$\begin{pmatrix} \text{Orthonormal basis set} \\ \text{for 2 qubits} \end{pmatrix} = \{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}. \tag{1.6}$$

More generally, if $N \geq 3$ qubits are considered, the Hilbert space of the composite system is denoted by $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_N$ which is a 2^N-dimensional Hilbert space. The natural orthonormal basis for this system is constructed as

$$\begin{pmatrix} \text{Orthonormal basis set} \\ \text{for N qubits} \end{pmatrix} = \{|0\cdots 00\rangle, |0\cdots 01\rangle, \cdots, |11\cdots 1\rangle\}. \tag{1.7}$$

This basis is usually called as the computational basis in quantum computation studies.

1.3 Density operator

Quantum mechanics is constructed by *measurements* performed on the quantum systems. The measurement outcomes are obtained with some *probabilities* [33]. Determining the probabilities corresponding to *observables* are achieved only by well-defined representations [32]. The difficulty arisen is that each state corresponding to different measurement outcomes have not only relative weights but also relative phases compared to each other. Therefore, if one has only statistical results about a quantum system, construction of the *quantum state vector* in the form of a *ket* may fail [34]. The knowledge of relative phases is also needed.

The set

$$\mathscr{E} = \{p_i, |\psi_i\rangle\} \tag{1.8}$$

is called the *ensemble of states* where each state $|\psi_i\rangle$ has the *fractional* probability p_i to be *found* in the ensemble. The difference between quantum probability and fractional probability is that while the former is *a posteriori* result *obtained* only by measurements performed on the system, the latter is *a priori* result *prepared* by *someone.* Another interpretation is that fractional probabilities is constructed in the brain of the *observer,* while quantum probabilities are ingrident of the *observable.*

To illustrate this, let an experimenter order 20 electrons from an imaginary company. Let 5 of them be in a spin-up state in x direction shown by $|\uparrow_x\rangle$ and other 15 be in a spin-down state in z direction shown by $|\downarrow_z\rangle$. The total system is constructed by a *single ket* such as $|\uparrow_x\rangle^{\otimes 5} \otimes |\downarrow_z\rangle^{\otimes 15}$, i.e., it is a pure state. However, the *state* of each electron can not be written in terms of a pure state like $\sqrt{0.25}\,|\uparrow_x\rangle + \sqrt{0.75}\,|\downarrow_z\rangle$. This is not so, because there is a relationship between $|\uparrow_x\rangle$ and $|\downarrow_z\rangle$ as

$$|\uparrow_x\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_z\rangle + |\downarrow_z\rangle\right) \tag{1.9}$$

meaning that $|\uparrow_x\rangle$ is not orthogonal to $|\downarrow_z\rangle$. Meanwhile, the possible state of type $\sqrt{0.25}\,|\uparrow_x\rangle + \sqrt{0.75}\,|\downarrow_z\rangle$ ignores the *relative phase* between the states $|\uparrow_x\rangle$ and $|\downarrow_z\rangle$. Morever, the probabilities 0.25 and 0.75 give different interpretations about the system. For example, the probability 0.25 is not the quantum probability when a possible measurement is performed on a single electron. This is because each electron is actually represented by a single ket, i.e., $|\uparrow_x\rangle$ or $|\downarrow_z\rangle$. Therefore, we need a different tool than *ket* or *wavefunction* to represent the states of individual quantum systems.

It is not obligatory that set $\{|\psi_i\rangle\}$ in the ensemble $\mathscr{E} = \{p_i, |\psi_i\rangle\}$ is an orthogonal set but all $|\psi_i\rangle$ must be normalized. If an ensemble for a quantum system is given, the density operator of the quantum system, which is developed independently by Landau [35] and von Neumann [36,37], can be formed as

$$\rho = \sum_{i=1}^{n} p_i \left|\psi_i\right\rangle \left\langle\psi_i\right| . \tag{1.10}$$

It is easily seen that if $|\psi_i\rangle$ is an N-dimensional column vector then the density matrix is $N \times N$ matrix because of the matrix multiplication of column vector $|\psi_i\rangle$ from the right with a row vector $\langle\psi_i|$. Note that n is the number of elements in $\mathscr{E} = \{p_i, |\psi_i\rangle\}$ and there is no obvious relation between the number n and the dimension N, so both $n \leq N$ and $N \leq n$ are possible [33].

If some ρ is given, it is easy to test whether it is a density matrix or not. There are two necessary and sufficient conditions for any ρ to be a density matrix:

1. ρ is positive; that is, for all $|\psi\rangle$, one has $\langle\psi|\rho|\psi\rangle \geq 0$ since

$$\begin{aligned} \langle\psi|\rho|\psi\rangle &= \sum_{i=1}^{n} p_i \langle\psi|\psi_i\rangle\langle\psi_i|\psi\rangle \\ &= \sum_{i=1}^{n} p_i \langle\psi|\psi_i\rangle\langle\psi|\psi_i\rangle^* \\ &= \sum_{i=1}^{n} p_i |\langle\psi|\psi_i\rangle|^2 \geq 0 \end{aligned} \tag{1.11}$$

   for all $|\psi\rangle$ because of the positivity of p_i and of the magnitude $|\langle\psi|\psi_i\rangle|$.

2. $\mathrm{tr}\rho = 1$ since

$$\begin{aligned} \mathrm{tr}\rho &= \sum_{j=1}^{N}\sum_{i=1}^{n} p_i \langle j|\psi_i\rangle\langle\psi_i|j\rangle \\ &= \sum_{i=1}^{n} p_i \sum_{j=1}^{N} |\langle j|\psi_i\rangle|^2 = \sum_{j=1}^{N} \left|\alpha_{ij}\right|^2 = 1 \end{aligned} \tag{1.12}$$

   where $\langle j|\psi_i\rangle = \alpha_{ij}$ for some orthonormal set $\{|j\rangle\}$ and since $|\psi_i\rangle$ can be written as a linear combination of $|j\rangle$ by means of the *completeness relation*

$$I_N = \sum_{j=1}^{N} |j\rangle\langle j| \tag{1.13}$$

   where I_N is the $N \times N$ *identity matrix.* Then,

$$|\psi_i\rangle = I_N |\psi_i\rangle = \left(\sum_{j=1}^{N} |j\rangle\langle j|\right)|\psi_i\rangle = \sum_{j=1}^{N} \langle j|\psi_i\rangle |j\rangle = \sum_{j=1}^{N} \alpha_{ij} |j\rangle \tag{1.14}$$

   for normalized $|\psi_i\rangle$ such that

$$\begin{aligned} \||\psi_i\rangle\| &= \sqrt{\langle\psi_i|\psi_i\rangle} = \sqrt{\sum_{j,k=1}^{N} \alpha_{ij}^*\alpha_{ik}\langle j|k\rangle} \\ &= \sqrt{\sum_{j,k=1}^{N} \alpha_{ij}^*\alpha_{ik}\delta_{jk}} = \sqrt{\sum_{j=1}^{N} \alpha_{ij}^*\alpha_{ij}} \\ &= \sqrt{\sum_{j=1}^{N} \left|\alpha_{ij}\right|^2} = 1 \end{aligned} \tag{1.15}$$

   where the orthonormality condition for $\{|j\rangle\}$ is $\langle j|k\rangle = \delta_{jk}$ where δ_{jk} is the *Kronecker delta.*

1.4 Mixed states versus pure states

In quantum mechanics, a pure state corresponds to a single *wavefunction*. If the state of a quantum system can be expressed as a *ket,* then it is called *a pure state*[33]. In other words, if in the ensemble given by Eq. (1.8), all possible states are identical, i.e., $|\psi_i\rangle = |\psi\rangle$ for all i, then this ensemble and the corresponding density matrix represents the pure state $|\psi\rangle$. In that case, $\rho = |\psi\rangle\langle\psi|$. However, when it is impossible to construct the state of the system as a *ket* [34], the state of the system is called *mixed*. In that case, $\rho = \sum_{i=1}^{n} p_i |\psi_i\rangle\langle\psi_i|$ where p_i is the probability of $|\psi_i\rangle$ in the ensemble where $\mathscr{E} = \{p_i, |\psi_i\rangle\}$. Alternative definitions of mixed states can easily be made since its analysis is very easy. For example, for a mixed state there are more than one non-zero eigenvalues of the corresponding density matrix.

Again, there is a frequently used condition for a given density matrix to be *mixed* or *pure.* The state is pure if

$$\mathrm{tr}\rho^2 = 1 \tag{1.16}$$

since if the system is in pure state, say $|\psi\rangle$, then

$$\begin{aligned} \mathrm{tr}(\rho^2) &= \mathrm{tr}\left\{(|\psi\rangle\langle\psi|)(|\psi\rangle\langle\psi|)\right\} \\ &= \mathrm{tr}\,(|\psi\rangle\langle\psi|) = \mathrm{tr}\rho = 1 \end{aligned} \tag{1.17}$$

and mixed if

$$\mathrm{tr}\rho^2 < 1 \tag{1.18}$$

since

$$\begin{aligned} \mathrm{tr}(\rho^2) &= \mathrm{tr}\left(\sum_{i=1}^{n} p_i |\psi_i\rangle\langle\psi_i|\right)^2 = \sum_{i,j=1}^{n} p_i p_j \left\langle \psi_j \middle| \psi_i \right\rangle \left\langle \psi_i \middle| \psi_j \right\rangle \\ &< \sum_{i,j=1}^{n} p_i p_j \, \| |\psi_i\rangle \|^2 \left\| |\psi_j\rangle \right\|^2 = \sum_{i=1}^{n} p_i \sum_{j=1}^{n} p_j = 1 \end{aligned} \tag{1.19}$$

where *the Cauchy-Schwartz inequality*[1] is used.

1.5 Partial trace

Consider a state ρ of a composite system formed by systems A, B, ..., N. All local measurements on A can be expressed by using a density matrix ρ_A defined by

$$\rho_A = \mathrm{tr}_{BC\cdots N}\rho \tag{1.20}$$

which is an operator that acts on A's Hilbert space. Here, the *trace* is taken over the whole system *excluding A.*

As an example, let the particles A and B be in the state

$$|\psi_{AB}\rangle = \frac{1}{\sqrt{2}}\left(|01\rangle - |10\rangle\right), \tag{1.21}$$

[1] Let $|v\rangle$ and $|w\rangle$ be two vectors , then the *Cauchy-Schwarz inequality* is

$$|\langle w\,|v\rangle|^2 \leq \langle w\,|w\rangle\langle v\,|v\rangle$$

where the equality is satisfied if only if $|v\rangle$ and $|w\rangle$ are parallel.

then the reduced density matrix ρ_A is calculated to be

$$\rho_A = \mathrm{tr}_B\left(|\psi_{AB}\rangle\langle\psi_{AB}|\right) \tag{1.22}$$

$$= \mathrm{tr}_B\left\{\frac{1}{2}\left[|01\rangle\langle 01| - |01\rangle\langle 10| - |10\rangle\langle 01| + |10\rangle\langle 10|\right]\right\} \tag{1.23}$$

$$\begin{aligned} &= \frac{1}{2}\{|0\rangle\langle 0|\,\mathrm{tr}\left(|1\rangle\langle 1|\right) - |0\rangle\langle 1|\,\mathrm{tr}\left(|1\rangle\langle 0|\right) \\ &\quad - |1\rangle\langle 0|\,\mathrm{tr}\left(|0\rangle\langle 1|\right) + |1\rangle\langle 1|\,\mathrm{tr}\left(|0\rangle\langle 0|\right)\} \end{aligned} \tag{1.24}$$

$$= \frac{1}{2}\left(|0\rangle\langle 0| + |1\rangle\langle 1|\right) = \frac{I}{2}$$

where I is the identity matrix. Note that in Eq. (1.24), the property of trace operation

$$\mathrm{tr}\left(|a\rangle\langle b|\right) = \langle b|a\rangle \tag{1.25}$$

is used for any quantum states $|a\rangle$ and $|b\rangle$, i.e.,

$$\mathrm{tr}(|0\rangle\langle 1|) = \langle 1|0\rangle = 0 = \mathrm{tr}(|1\rangle\langle 0|) = \langle 0|1\rangle \tag{1.26}$$

and

$$\mathrm{tr}(|0\rangle\langle 0|) = \langle 0|0\rangle = 1 = \mathrm{tr}(|1\rangle\langle 1|) = \langle 1|1\rangle\,. \tag{1.27}$$

1.6 Entanglement

Let the pure state of a composite system AB be $|\psi_{AB}\rangle$ where the corresponding Hilbert spaces being $\mathcal{H}_A$ and $\mathcal{H}_B$. Let m and n be the dimensions of the respective spaces. The state $|\psi_{AB}\rangle$ can be decomposed as

$$|\psi_{AB}\rangle = \sum_{i=1}^{n_\psi} \sqrt{\mu_i}\,|i_A\rangle \otimes |i_B\rangle \qquad (\text{here } n_\psi \leq \min(m,n)) \tag{1.28}$$

where $\{|i_A\rangle\}$ forms an orthonormal set in $\mathcal{H}_A$ and $\{|i_B\rangle\}$ forms an orthonormal set in $\mathcal{H}_B$. Here the real-valued coefficients $\sqrt{\mu_i}$ are called the Schmidt coefficients, after Erhard Schmidt[38]. The numbers μ_i satisfy the following normalization condition

$$\sum_i^{n_\psi} \mu_i = 1 \tag{1.29}$$

in which n_ψ is called the Schmidt rank of the state $|\psi_{AB}\rangle$. It is easy to show that the numbers μ_i are eigenvalues of both of the reduced density matrices ρ_A and ρ_B with the corresponding eigenvectors being $|i_A\rangle$ and $|i_B\rangle$, respectively. This result stems from the fact that density matrices are positive operators which have spectral decompositions into their orthonormal set of eigenvectors of which diagonal elements are corresponding to their eigenvalues. Also, since they are positive and $\mathrm{tr}\rho_A = \mathrm{tr}\rho_B = 1$, they satisfy the Schmidt's condition on positivity and reality of μ_i and their normalization such that $\sum_i^{n_\psi} \mu_i = 1$. Hence, the spectral decompositions of ρ_A and ρ_B are obtained as the following:

$$\begin{aligned} \rho_A &= \mathrm{tr}_B\left(|\psi_{AB}\rangle\langle\psi_{AB}|\right) = \sum_{i,j=1}^{n_\psi} \sqrt{\mu_i\mu_j}\,|i_A\rangle\langle j_A|\,\mathrm{tr}\left(|i_B\rangle\langle j_B|\right) \\ &= \sum_{i,j=1}^{n_\psi} \sqrt{\mu_i\mu_j}\,|i_A\rangle\langle j_A|\langle j_B|\,i_B\rangle \\ &= \sum_{i=1}^{n_\psi} \mu_i\,|i_A\rangle\langle i_A| \end{aligned} \tag{1.30}$$

since $|i_B\rangle$'s form an orthonormal basis set, i.e., $\langle j_B | i_B\rangle = \delta_{ij}$. With similar calculations, ρ_B is obtained as

$$\rho_B = \mathrm{tr}_A \left(|\psi_{AB}\rangle \langle\psi_{AB}|\right) = \sum_{i=1}^{n_\psi} \mu_i \, |i_B\rangle \langle i_B| \, . \tag{1.31}$$

Accordingly, one can say that μ_i's are eigenvalues of ρ_A and ρ_B with the corresponding orthonormal set of eigenvectors $|i_A\rangle$ and $|i_B\rangle$, respectively [36,39].

Let two spin-1/2 particles labelled by A and B physically interact for some time in the past. Later, let A and B be get separated until this interaction terminates. Then, let Alice (A) be given one of them and Bob (B) be given the other. Despite the absence of interaction, there is a very special situation where the quantum states of individual systems are no longer represented *independently* of each other. This phenomenon is known as *quantum entanglement*, a name which is coined by E. Schrödinger [40]. The simplest entangled state is the singlet state formed between two spin-1/2 particles. In terms of Eq. (1.6), this *maximally entangled* state has the form

$$|\psi_{AB}\rangle = \frac{1}{\sqrt{2}} \left(|01\rangle - |10\rangle\right) \tag{1.32}$$

where $|0\rangle = |\uparrow_z\rangle$ and $|1\rangle = |\downarrow_z\rangle$ in this case. Particles in such entangled states are called *EPR pairs* by Einsten-Podolsky-Rosen [1]. An orthonormal basis formed by maximally entangled states can be found, for example the set of vectors $\left|\beta_{xy}\right\rangle$ where

$$\left|\beta_{xy}\right\rangle = \frac{1}{\sqrt{2}} \left(|0, y\rangle + (-1)^x \, |1, \bar{y}\rangle\right) \tag{1.33}$$

where $\bar{y}$ is the negation of y; for example $\left|\bar{0}\right\rangle = |1\rangle$ and $\left|\bar{1}\right\rangle = |0\rangle$. The set of vectors $\{\left|\beta_{xy}\right\rangle\}$ forms an orthonormal basis of the 2×2 dimensional Hilbert space of two qubits[36].

The states in Eq. (1.33) are called *entangled* since they can not be written in a *product* form like $|a\rangle_A \otimes |b\rangle_B$. This state leads to some extraordinary and even unimaginable applications of entanglement in quantum information and computation. To see this, consider two parties Alice and Bob sharing particles A and B which is in an entangled state of the form Eq. (1.33). Separate the particles so that there is no *interaction* between the particles. Nevertheless, all the *local* operations performed only by Alice on her qubit can change the state of the qubit B. These local operations directly affect the results of the local operations on the qubit B performed by Bob. This is because the state of each qubit can not be expressed separately.

In the language of the Schmidt decomposition, a bipartite pure state is entangled iff its Schmidt rank is 2 or more and unentangled if its Schmidt rank is 1. Looking at the Eq. (1.23) for $\rho_A = \frac{1}{2} \left(|0\rangle \langle 0| + |1\rangle \langle 1|\right)$ in the case of $|\psi_{AB}\rangle = \left(|01\rangle - |10\rangle\right) / \sqrt{2}$, the Schmidt rank is $n_\psi = 2$, i.e., $|\psi_{AB}\rangle$ is entangled. Also, note that eigenvectors $\{|0\rangle , |1\rangle\}$ of ρ_A corresponds to the positive eigenvalues $\mu_{1,2} = \frac{1}{2}$. These eigenvalues satisfy the Eq. (1.29) since $\sum_i^2 \mu_i = 1$. Now, consider the product state $|\psi_{AB}\rangle = |00\rangle$, then $\rho_A = |0\rangle \langle 0|$. Its Schmidt rank is 1, therefore it is unentangled.

1.7 W and GHZ class entangled states of three qubits

In a similar manner with Sec. 1.6, when more than two qubits are involved, then entangled states of very different kinds can be obtained [6-9,39,42-53]. However, Bennett and DaVincenzo have argued that despite a lot of work on multipartite entanglement, it still remains a mystery. Thus, they can not be treated as in the case of bipartite entanglement [51]. In the case of three qubit system, there is a pure state

$$|W\rangle = \frac{|100\rangle + |010\rangle + |001\rangle}{\sqrt{3}} \tag{1.34}$$

which is also known as the W state. This state is closely related to the general "W type" state of three or more particles which are described as follows: for p qubits

$$|\Psi_W\rangle = \sqrt{x_0}\,|\mathbf{0}\rangle + \sum_{k=1}^{p} \sqrt{x_k}\,|\mathbf{1}_k\rangle \text{ for } k = 1, 2, \cdots, p \tag{1.35}$$

where $|\mathbf{0}\rangle = |00\cdots 0\rangle$ and $|\mathbf{1}_k\rangle$ is the state when the k^{th} qubit is in state 1 and the rest is in state 0 [50]. In other words, Bruß states that a geniune W state is constructed by a superposition of the parties which are in cyclic permutations of each other and one party should be in excited state [47]. Also, x_0 and all x_k are real and positive that obey the sum (or normalization)

$$x_0 + \sum_{k=1}^{p} x_k = 1. \tag{1.36}$$

Note that $|W\rangle$ defined by Eq. (1.34) can not be written in a product state like

$$|W\rangle \neq |a_1\rangle \otimes |a_2\rangle \otimes |a_3\rangle \tag{1.37}$$

so $|W\rangle$ is necessarily an entangled state.

Another type of tripartite entangled state can be obtained as follows

$$|GHZ\rangle = \frac{|000\rangle + |111\rangle}{\sqrt{2}} \tag{1.38}$$

which is known as the Greenberger-Horne-Zeilinger (GHZ) state[43]. This is closely related to the "GHZ-type" entangled state which is defined as

$$|\Psi\rangle_{GHZ} = \frac{1}{N}\left(|0\rangle^{\otimes p} + z\,|\beta_1\rangle \otimes |\beta_2\rangle \otimes \cdots \otimes \left|\beta_p\right\rangle\right) \tag{1.39}$$

where p is the number of parties involved, N is normalization constant, z is an arbitrary complex number. It is also known as p-particle Cat (p-Cat) state because of Schrödinger's cat [42] when $|\beta_k\rangle = |1\rangle$ for all k. Also, note that each state $|\beta_k\rangle$ in Eq. (1.39) has the form

$$|\beta_k\rangle = c_k\,|0\rangle + s_k\,|1\rangle \equiv \begin{pmatrix} c_k \\ s_k \end{pmatrix} \tag{1.40}$$

for each k with the obvious condition that $s_k \neq 0$ for all k at the same time. Here, note that all $|\beta_k\rangle$'s are unit vector and c_k and s_k can be seen as *cosine* and *sine* functions of some real angle θ_k, respectively, then it is obvious that

$$c_k^2 + s_k^2 = 1 \tag{1.41}$$

for all k's. Again, it is clear that $|\Psi\rangle_{GHZ}$ in Eq. (1.39) can not be written as a product state such that

$$|\Psi\rangle_{GHZ} \neq |a_1\rangle \otimes |a_2\rangle \otimes \cdots \otimes \left|a_p\right\rangle , \tag{1.42}$$

if at least two sines are non-zero.

1.8 SLOCC equivalence of pure states

Consider two possible multipartite states $|\psi\rangle$ and $|\phi\rangle$ of N systems (particles) *A, B, ..., N. Stochastic local operations assisted with classical communications (SLOCC)* transformations for these states are defined as follows: $|\psi\rangle$ is *stochastically reducible* to $|\phi\rangle$ (shown by $|\psi\rangle \underset{SLOCC}{\longrightarrow} |\phi\rangle$) if there are local operators $A, B, \ldots, N$ such that

$$|\phi\rangle = A \otimes B \otimes \cdots \otimes N \, |\psi\rangle \, . \tag{1.43}$$

Also, $|\psi\rangle$ is *stochastically equivalent* to $|\phi\rangle$ or *SLOCC equivalent* to $|\phi\rangle$ (shown by $|\psi\rangle \underset{SLOCC}{\sim} |\phi\rangle$) if $|\psi\rangle \underset{SLOCC}{\longrightarrow} |\phi\rangle$ and $|\phi\rangle \underset{SLOCC}{\longrightarrow} |\psi\rangle$. If we can find *invertible local operators* (ILO), *A, B, ..., N,* transforming the state $|\psi\rangle$ into the state $|\phi\rangle$, then $|\psi\rangle$ is said to be equivalent to $|\phi\rangle$ under *SLOCC* transformations:

$$|\psi\rangle \underset{SLOCC}{\sim} |\phi\rangle \text{ iff } |\phi\rangle = A \otimes B \otimes \cdots \otimes N \, |\psi\rangle \quad \text{for some invertible } A, B, \ldots, N. \tag{1.44}$$

It is also true that

$$|\psi\rangle = A^{-1} \otimes B^{-1} \otimes \cdots \otimes N^{-1} \, |\phi\rangle \tag{1.45}$$

where A^{-1}, B^{-1},...,N^{-1} are the inverses of the ILO's *A, B, ..., N,* respectively [39].

It can easily be shown that if $|\psi\rangle \underset{SLOCC}{\sim} |\phi\rangle$, then ranks of the reduced density matrices of the corresponding local parties are equal [39], i.e.,

$$r\left(\rho_k^{\psi}\right) = r\left(\rho_k^{\phi}\right) \text{ for } k = A, B, \cdots, N. \tag{1.46}$$

In Chap. 4, SLOCC classes for rank 2 mixed states of two qubits are constructed.

CHAPTER 2

CONCURRENCE

2.1 Partly entangled bipartite pure state

Suppose that the particles A and B are in the "partially" entangled bipartite pure state $|\psi\rangle_{AB}$

$$|\psi\rangle_{AB} = \alpha\,|00\rangle + \beta\,|11\rangle \tag{2.1}$$

where α and β are some arbitrary constants satisfying the normalization condition $|\alpha|^2 + |\beta|^2 = 1$.

Bennett *et. al.* [42] have shown that, for the asymptotic transformations of pure bipartite entangled states, there is a single measure of entanglement, which is defined as the *von Neumann entropy* of the reduced density matrices of the state as follows

$$E\,(\psi_{AB}) = -\mathrm{tr}\,(\rho_A \log_2 \rho_A) = -\mathrm{tr}\,(\rho_B \log_2 \rho_B) \tag{2.2}$$

where ρ_A and ρ_B are the reduced density matrices of the parties A and B, respectively. Then, for the state $|\psi\rangle_{AB}$ given by the Eq. (2.1), the reduced density matrix ρ_A of A is calculated to be

$$\begin{aligned} \rho_A &= \mathrm{tr}_B\,(|\psi\rangle\,\langle\psi|)_{AB} = |\alpha|^2\,|0\rangle\,\langle 0| + |\beta|^2\,|1\rangle\,\langle 1| \\ &= \begin{pmatrix} |\alpha|^2 & 0 \\ 0 & |\beta|^2 \end{pmatrix}. \end{aligned} \tag{2.3}$$

Putting Eq. (2.3) into Eq. (2.2) results in the entanglement

$$\begin{aligned} E\,(\psi_{AB}) &= -\mathrm{tr}\begin{pmatrix} |\alpha|^2 \log_2 |\alpha|^2 & 0 \\ 0 & |\beta|^2 \log_2 |\beta|^2 \end{pmatrix} \\ &= -\,|\alpha|^2 \log_2 |\alpha|^2 - |\beta|^2 \log_2 |\beta|^2\,. \end{aligned} \tag{2.4}$$

A related entanglement measure which appears to be useful in the discussion of bipartite entanglement of two qubits is the concurrence. The value of the concurrence for the pure state given in Eq. (2.1) is simply equal to

$$C\,(\psi_{AB}) = 2\,|\alpha|\,|\beta| = 2\,\sqrt{\det \rho_A} = 2\,\sqrt{\det \rho_B}. \tag{2.5}$$

The amount of entanglement E for the pure state in Eq. (2.1) can be expressed as

$$E(C) = h\left(\frac{1 + \sqrt{1 - C^2}}{2}\right). \tag{2.6}$$

Here, $h(x)$ is the function

$$h(x) = -x \log_2 x - (1 - x) \log_2 (1 - x). \tag{2.7}$$

The concurrence can also be defined for mixed states of two qubits as well [54], however, this time the calculation is more involved. In the following sections, we describe the calculation method and compute the value of C for rank 2 mixed states of two qubits.

2.1.1 Pure state concurrence $C(\psi)$

Concurrence of a pure state $|\psi\rangle = |\psi\rangle_{AB}$ of two qubits can be expressed as

$$C(\psi) = \left|\langle\psi \mid \tilde{\psi}\rangle\right| \tag{2.8}$$

where $|\tilde{\psi}\rangle$ is the *spin flip state* for $|\psi\rangle$ calculated by the formula

$$|\tilde{\psi}\rangle = \sigma_y^{\otimes 2}|\psi^*\rangle \tag{2.9}$$

where $|\psi^*\rangle$ is the complex conjugate of $|\psi\rangle$ in the computational basis. Here, $\sigma_y^{\otimes 2}$ is given by $\sigma_y^{\otimes 2} = \sigma_y \otimes \sigma_y$ for the Pauli operator $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ in the computational basis set $\{|0\rangle, |1\rangle\}$. It acts separately on each qubit as $\sigma_y|0\rangle = i|1\rangle$ and $\sigma_y|1\rangle = -i|0\rangle$. Then,

$$\sigma_y^{\otimes 2}|00\rangle = -|11\rangle \text{ and } \sigma_y^{\otimes 2}|11\rangle = -|00\rangle . \tag{2.10}$$

Now, applying these operations on Eq. (2.1), the spin flip state is found as

$$|\tilde{\psi}\rangle = -\alpha^*|11\rangle - \beta^*|00\rangle . \tag{2.11}$$

Then, concurrence is calculated to be

$$C(\psi_{AB}) = 2|\alpha||\beta| . \tag{2.12}$$

Notice that the concurrence of a maximally entangled state given by Eq. (1.32) is found as $C = 1$ since $\alpha = -\beta = 1/\sqrt{2}$. However, the concurrence of any product state like $|00\rangle$ is found 0 since $\beta = 0$. Therefore, concurrence is some kind of a measure of entanglement, i.e., more concurrence means a more entangled state. Note that $E = E(C)$ in Eq. (2.6) is a monotonically increasing function of C, which also takes values in the interval $(0, 1)$. Hence, by the same token, E is a similar kind of measure.

2.1.2 Concurrence of a mixed state

For a mixed state, the concurrence is defined in an elaborate way. The R *matrix* of a mixed state $\rho = \rho_{AB}$ of two qubits is defined by

$$R(\rho) = \sqrt{\sqrt{\rho}\tilde{\rho}\sqrt{\rho}} \tag{2.13}$$

where $\tilde{\rho}$ is the spin flip state given by

$$\tilde{\rho} = \sigma_y^{\otimes 2}\rho^*\sigma_y^{\otimes 2}, \tag{2.14}$$

where ρ^* is obtained by taking the complex conjugate of ρ in the computational basis. Let the eigenvalues of $R(\rho)$ be

$$\text{Eigenvalues of } R(\rho) = \{\lambda_1, \lambda_2, \lambda_3, \lambda_4\} \tag{2.15}$$

in *non-increasing order*, i.e., $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$. Then the concurrence is calculated as

$$C(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\} . \tag{2.16}$$

For any pure state $|\psi\rangle$, the density matrix ρ is $\rho = |\psi\rangle\langle\psi|$ and the spin-flipped state $\tilde{\rho}$ is $\tilde{\rho} = |\tilde{\psi}\rangle\langle\tilde{\psi}|$. Note that $\rho = |\psi\rangle\langle\psi|$ is a four dimensional density matrix and is already *diagonal* or *spectrally decomposed* (i.e. a *projector*[1]) with eigenvalue 1 for the eigenstate $|\psi\rangle$ and 0 for the other three *mutually orthonormal eigenstates*, which all form an orthonormal basis. Then, the square root function $\sqrt{\cdots}$ can operate directly on ρ as $\sqrt{\rho} = \sqrt{1}\,|\psi\rangle\langle\psi| = \rho$. Therefore, using the Dirac representations for $\sqrt{\rho}$ and $\tilde{\rho}$, $R(\rho)$ is found as

$$\begin{aligned} R(\rho) &= \sqrt{\sqrt{\rho}\tilde{\rho}\sqrt{\rho}} = \sqrt{(|\psi\rangle\langle\psi|)(|\tilde{\psi}\rangle\langle\tilde{\psi}|)(|\psi\rangle\langle\psi|)} \\ &= \left|\langle\psi \mid \tilde{\psi}\rangle\right|\rho = C(\psi)\rho \end{aligned} \tag{2.17}$$

which is already in its spectral form like ρ whose one eigenvalue is 1 and other three are 0. Then the eigenvalues, in of $R(\rho)$ are

$$\{\lambda_1, \lambda_2, \lambda_3, \lambda_4\} = \{C(\psi), 0, 0, 0\}. \tag{2.18}$$

Thus, using Eq. (2.16), the concurrence $C(\rho_{AB})$ is

$$C(\rho_{AB}) = C(\psi_{AB}) = 2|\alpha||\beta|. \tag{2.19}$$

As a result, the Eq. (2.16) of the concurrence for mixed states can also be used to find the concurrence of a pure state which is a rank 1 mixed state.

2.1.3 Eigenvalues of $\rho\tilde{\rho}$

In this section, instead of finding the eigenvalues λ of $R(\rho)$, the square roots of the eigenvalues γ of the matrix multiplication $\rho\tilde{\rho}$

$$\text{Eigenvalues of } \rho\tilde{\rho} = \{\gamma_1, \gamma_2, \gamma_3, \gamma_4\} \tag{2.20}$$

are used to find the concurrence so that

$$C(\rho) = \max\{0, \sqrt{\gamma_1} - \sqrt{\gamma_2} - \sqrt{\gamma_3} - \sqrt{\gamma_4}\}. \tag{2.21}$$

This can be shown as follows. It is a well-known result in linear algebra that similar matrices have the same set of eigenvalues. For two matrices A and B, the matrix AB is similar to

$$A^{-1}(AB)A = BA. \tag{2.22}$$

Hence, the set of eigenvalues of AB and BA are identical. By continuity of the dependence of eigenvalues on matrices, the same conclusion holds even when A and B are non-invertible. Therefore, $R^2 = \sqrt{\rho}\tilde{\rho}\sqrt{\rho}$ and $\sqrt{\rho}\sqrt{\rho}\tilde{\rho} = \rho\tilde{\rho}$ are isospectral. Note that $\rho\tilde{\rho}$ is not Hermitian. But, since R^2 is a positive definite and hermitian, the eigenvalues of $\rho\tilde{\rho}$ are real and non-negative.

In conclusion, concurrence of a bipartite pure state can be found by the Eq. (2.8) for pure states, by $R(\rho)$ in Eq. (2.13), and also by direct multiplication $\rho\tilde{\rho}$ developed for rank 2 mixed states.

2.2 Bipartite mixed states with matrix rank 2

Consider a mixed state $\rho = \rho_{AB}$ of two qubits A and B. Let us suppose that ρ_{AB} has matrix rank 2, i.e., it has only 2 non-zero eigenvalues. Let us suppose that its eigenvalues are q_i and eigenvectors are

[1] Any projector has eigenvalues 1 and 0.

$|\psi_i\rangle_{AB}$ ($i = 1, 2$). Therefore, we have

$$\rho_{AB} = \sum_{i=1}^{2} q_i \left(|\psi_i\rangle \langle\psi_i|\right)_{AB} . \tag{2.23}$$

For some problems, it is useful to think of AB as being entangled to a hypothetical system C such that ABC are in a pure state $|\Psi\rangle_{ABC}$ and $\rho_{AB} = \mathrm{tr}_C \left(|\Psi\rangle \langle\Psi|\right)_{ABC}$. The state $|\Psi\rangle_{ABC}$ is usually termed a purification of ρ_{AB}. A straightforward purification of Eq. (2.23) is obtained as

$$|\Psi\rangle_{ABC} = \sqrt{q_1}\, |\psi_1\rangle_{AB} \otimes |0\rangle_C + \sqrt{q_2}\, |\psi_2\rangle_{AB} \otimes |1\rangle_C . \tag{2.24}$$

Therefore, $|\Psi\rangle_{ABC}$ is a pure state of 3 qubits when ρ_{AB} has matrix rank 2. The classification by Dür *et. al.* [39] of pure states of 3 qubits enables us to classify the rank 2 mixed states of 2 qubits.

In the following, we will consider the two types of mixed states ρ_{AB} separately. Namely, those states where purification is of W class and those ones whose purification is of GHZ class. Using well-known representations of these pure states, we will obtain the concurrence of the mixed state ρ_{AB}.

2.2.1 The case where the purification is of W class

Consider three qubits A, B and C. Let ABC be in a 3-partite W-type entangled state $|\Psi\rangle_{ABC}$ defined by Eq. (1.35) for $p = 3$ such that

$$|\Psi\rangle_{ABC} = \sqrt{x_0}\, |000\rangle + \sqrt{x_1}\, |100\rangle + \sqrt{x_2}\, |010\rangle + \sqrt{x_3}\, |001\rangle \tag{2.25}$$

where the coefficients x_0 and each x_k for $k = 1, 2, 3$ are some *positive real* numbers which satisfy

$$x_0 + \sum_{k=1}^{3} x_k = 1. \tag{2.26}$$

In the following sections, from the pure state $|\Psi\rangle_{ABC}$, first the density matrix of the composite system ABC, then, the reduced density matrix of the subsystem AB are calculated. Finally, it is shown that there is an entanglement between the qubits belonging to A and B by using Eq. (2.16) for concurrence derived for mixed states of 2 qubits. For the reader to easily follow the calculations, it is more convenient to separate $|\Psi\rangle_{ABC}$ as AB-C like in the purification of ρ_{AB} given by Eq. (2.16) as follows

$$|\Psi\rangle_{ABC} = \left(\sqrt{x_0}\, |00\rangle + \sqrt{x_1}\, |10\rangle + \sqrt{x_2}\, |01\rangle\right)_{AB} \otimes |0\rangle_C + \sqrt{x_3}\, |00\rangle \otimes |1\rangle_C \tag{2.27}$$

with

$$|\psi_1\rangle_{AB} = \sqrt{x_0}\, |00\rangle + \sqrt{x_1}\, |10\rangle + \sqrt{x_2}\, |01\rangle \;\text{ and }\; |\psi_2\rangle_{AB} = \sqrt{x_3}\, |00\rangle \tag{2.28}$$

which are unnormalized vectors. Here, also $q_1 = 1$ and $q_2 = 1$ which are nothing to do with the eigenvalues given by Eq. (2.23). The density operator ρ^W_{ABC} of ABC system is obtained then

$$\begin{aligned}
\rho^W_{ABC} &= \left(|\Psi\rangle \langle\Psi|\right)_{ABC} \\
&= \left(|\psi_1\rangle \langle\psi_1|\right)_{AB} \otimes \left(|0\rangle \langle 0|\right)_C + \left(|\psi_1\rangle \langle\psi_2|\right)_{AB} \otimes \left(|0\rangle \langle 1|\right)_C \\
&\quad + \left(|\psi_2\rangle \langle\psi_1|\right)_{AB} \otimes \left(|1\rangle \langle 0|\right)_C + \left(|\psi_2\rangle \langle\psi_2|\right)_{AB} \otimes \left(|1\rangle \langle 1|\right)_C .
\end{aligned}$$

Therefore the reduced density matrix ρ^W_{AB} is

$$\rho^W_{AB} = \mathrm{tr}_C \rho^W_{ABC} = \left(|\psi_1\rangle \langle\psi_1|\right)_{AB} + \left(|\psi_2\rangle \langle\psi_2|\right)_{AB} . \tag{2.29}$$

Here, in the intermediate steps, Eqs. (1.26) and (1.27) are used for the trace operations. On the other hand, ρ_{AB}^{W} can be represented in a matrix form in the computational basis set for two qubits substituting $|\psi_1\rangle_{AB}$ and $|\psi_2\rangle_{AB}$ defined by Eq. (2.28) into Eq. (2.29) as

$$\rho_{AB}^{W} = \begin{pmatrix} x_0 + x_3 & \sqrt{x_0 x_2} & \sqrt{x_0 x_1} & 0 \\ \sqrt{x_0 x_2} & x_2 & \sqrt{x_1 x_2} & 0 \\ \sqrt{x_0 x_1} & \sqrt{x_1 x_2} & x_1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{2.30}$$

Since x_k's in Eq. (2.25) are real for all k, then ρ_{AB}^{W} is a real matrix. Also, the tensor product $\sigma_y^{\otimes 2}$ is obtained in a matrix representation as

$$\sigma_y^{\otimes 2} = \begin{pmatrix} 0 & -i\sigma_y \\ i\sigma_y & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}. \tag{2.31}$$

Thus, the spin flip state is easily calculated by matrix multiplication as

$$\tilde{\rho}_{AB}^{W} = \sigma_y^{\otimes 2} \rho_{AB}^{W*} \sigma_y^{\otimes 2} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & x_1 & \sqrt{x_1 x_2} & -\sqrt{x_0 x_1} \\ 0 & \sqrt{x_1 x_2} & x_2 & -\sqrt{x_0 x_2} \\ 0 & -\sqrt{x_0 x_1} & -\sqrt{x_0 x_2} & (x_0 + x_3) \end{pmatrix} \tag{2.32}$$

in the computational basis set. The matrix multiplication of ρ_{AB}^{W} with $\tilde{\rho}_{AB}^{W}$ is then

$$\rho_{AB}^{W} \tilde{\rho}_{AB}^{W} = \begin{pmatrix} 0 & 2x_1 \sqrt{x_0 x_2} & 2x_2 \sqrt{x_0 x_1} & -2x_0 \sqrt{x_1 x_2} \\ 0 & 2x_1 x_2 & 2x_2 \sqrt{x_1 x_2} & -2x_2 \sqrt{x_0 x_1} \\ 0 & 2x_1 \sqrt{x_1 x_2} & 2x_1 x_2 & -2x_1 \sqrt{x_0 x_2} \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{2.33}$$

Then, the eigenvalues γ_i of the matrix $\rho_{AB}^{W} \tilde{\rho}_{AB}^{W}$ can easily be calculated since they are the roots of the *characteristic equation*

$$c(\gamma) = \gamma^3 (\gamma - 4x_1 x_2) \tag{2.34}$$

whose solution, i.e. $c(\gamma) = 0$, gives the set of eigenvalues γ_i as

$$\{\gamma_1, \gamma_2, \gamma_3, \gamma_4\} = \{4x_1 x_2, 0, 0, 0\} \tag{2.35}$$

in non-increasing order. Square root of the eigenvalues γ_i of $\rho_{AB}^{W} \tilde{\rho}_{AB}^{W}$ gives the set of eigenvalues λ_i of $R\left(\rho_{AB}^{W}\right)$ as

$$\{\lambda_1, \lambda_2, \lambda_3, \lambda_4\} = \left\{2\sqrt{x_1 x_2}, 0, 0, 0\right\} \tag{2.36}$$

in non-increasing order. Substitute the eigenvalues λ_i given by Eq. (2.36) into Eq. (2.16) for the concurrence to get

$$C\left(\rho_{AB}^{W}\right) = 2\sqrt{x_1 x_2} \tag{2.37}$$

since both x_1 and x_2 are positive numbers.

2.2.2 The case where the purification is of GHZ class

Start with the general form given by Eq. (1.39) for *p-partite* GHZ-type state. Let $p = 3$ so that three qubits A, B, and C are in the following tripartite GHZ-type entangled state

$$|\Psi\rangle_{ABC} = \frac{1}{N}\left(|000\rangle + z\,|\beta_1\beta_2\beta_3\rangle\right) \tag{2.38}$$

where N represents the normalization constant, and z is an arbitrary complex number. Here, $|\beta_i\rangle$'s are some arbitrary unit state vectors defined by Eq. (1.40). In order for $|\Psi\rangle_{ABC}$ to be a unit vector, the normalization constant N should be equal to the norm of $|000\rangle + z\,|\beta_1\beta_2\beta_3\rangle$ such that

$$N = \sqrt{(\langle 000| + z^*\,\langle\beta_1\beta_2\beta_3|)\,(|000\rangle + z\,|\beta_1\beta_2\beta_3\rangle)}. \tag{2.39}$$

To simplify the calculations note that $\langle 0|\,\beta_i\rangle = c_i$ and $\langle 1|\,\beta_i\rangle = s_i$ and substitute them into Eq. (2.39) to obtain

$$N = \sqrt{1 + 2c_1c_2c_3\Re(z) + |z|^2} \tag{2.40}$$

where $\Re(z) = (z + z^*)/2$ is the real part of z.

While it was convenient to deal with the matrix representations for the example of W-type in the Sec. 2.2.1, it is not in here. Due to the fact that ρ^{GHZ}_{ABC} contains too many parameters, another approach is called for. The following quantum mechanical tool is developed for faster calculations instead of the slower matrix method.

Firstly, write $|\Psi\rangle_{ABC}$ given by Eq. (2.38) as the sum of the tensor products of the subsystem AB and C as follows

$$|\Psi\rangle_{ABC} = |a_1\rangle_{AB} \otimes |0\rangle_C + |a_2\rangle_{AB} \otimes |1\rangle_C \tag{2.41}$$

$$= \frac{1}{N}\left(|00\rangle + zc_3\,|\beta_1\beta_2\rangle\right)_{AB} \otimes |0\rangle_C + \frac{zs_3}{N}\,|\beta_1\beta_2\rangle_{AB} \otimes |1\rangle_C\,. \tag{2.42}$$

Then, we note that

$$|a_1\rangle_{AB} = \frac{1}{N}\left(|00\rangle + zc_3\,|\beta_1\beta_2\rangle\right) \text{ and } |a_2\rangle_{AB} = \frac{zs_3}{N}\,|\beta_1\beta_2\rangle\,. \tag{2.43}$$

Secondly, $|a_1\rangle_{AB}$ and $|a_2\rangle_{AB}$ can be given a matrix representation in the computational basis set. The tensor product $|\beta_1\beta_2\rangle$ is obtained as

$$|\beta_1\beta_2\rangle = \begin{pmatrix} c_1c_2 \\ c_1s_2 \\ s_1c_2 \\ s_1s_2 \end{pmatrix} \tag{2.44}$$

where the column vector representations of $|\beta_1\rangle_A$ and $|\beta_2\rangle_B$ given by Eq. (1.40) are used in Eq. (2.44).

Finally, substituting Eq. (2.44) for $|\beta_1\beta_2\rangle$ and Eq. (1.5) for $|00\rangle$ into Eq. (2.43), $|a_1\rangle_{AB}$ and $|a_2\rangle_{AB}$ have the column vector representations

$$|a_1\rangle_{AB} = \frac{1}{N}\begin{pmatrix} 1 + zc_1c_2c_3 \\ zc_1s_2c_3 \\ zs_1c_2c_3 \\ zs_1s_2c_3 \end{pmatrix}, \quad |a_2\rangle_{AB} = \frac{zs_3}{N}\begin{pmatrix} c_1c_2 \\ c_1s_2 \\ s_1c_2 \\ s_1s_2 \end{pmatrix}. \tag{2.45}$$

Besides, by normalization of Eq. (2.41) and with the abbreviation $|a_i\rangle = |a_i\rangle_{AB}$ note that

$$\| |\Psi\rangle_{ABC} \|^2 = 1 = \langle a_1 | \, a_1 \rangle + \langle a_2 | \, a_2 \rangle = \sum_{i=1}^{2} \| |a_i\rangle \|^2 \tag{2.46}$$

of which use is made repeatedly throughout the thesis.

Thus, the reduced density matrix ρ_{AB}^{GHZ} of AB is found as

$$\rho_{AB}^{GHZ} = tr_C \left(|\Psi\rangle \langle \Psi| \right)_{ABC} = |a_1\rangle \langle a_1| + |a_2\rangle \langle a_2| = \sum_{i=1}^{2} |a_i\rangle \langle a_i| \tag{2.47}$$

which is a rank 2 mixed state. Alternatively, if ρ_{AB}^{GHZ} is written in a matrix representation putting Eq. (2.45) in Eq. (2.47), the columns of the 4×4 matrix ρ_{AB}^{GHZ} will be calculated as

$$\{1^{st} \text{ Col.}\} = \frac{1}{N^2} \begin{pmatrix} 1 + (|z|\, c_1 c_2)^2 + 2 c_1 c_2 c_3 \Re(z) \\ (|z|\, c_1)^2 c_2 s_2 + 2 c_1 s_2 c_3 \Re(z) \\ (|z|\, c_2)^2 c_1 s_1 + 2 s_1 c_2 c_3 \Re(z) \\ |z|^2\, c_1 s_1 c_2 s_2 + 2 s_1 s_2 c_3 \Re(z) \end{pmatrix}, \tag{2.48}$$

$$\left\{2^{nd} \text{ Col.}\right\} = \frac{1}{N^2} \begin{pmatrix} (|z|\, c_1)^2 c_2 s_2 + 2 c_1 s_2 c_3 \Re(z) \\ (|z|\, c_1 s_2)^2 \\ |z|^2\, c_1 s_1 c_2 s_2 \\ (|z|\, s_2)^2 s_1 c_2 \end{pmatrix}, \tag{2.49}$$

$$\left\{3^{rd} \text{ Col.}\right\} = \frac{1}{N^2} \begin{pmatrix} (|z|\, c_2)^2 c_1 s_1 + 2 s_1 c_2 c_3 \Re(z) \\ |z|^2\, c_1 s_1 c_2 s_2 \\ (|z|\, s_1 c_2)^2 \\ (|z|\, s_1)^2 c_2 s_2 \end{pmatrix}, \tag{2.50}$$

$$\left\{4^{th} \text{ Col.}\right\} = \frac{1}{N^2} \begin{pmatrix} |z|^2\, c_1 s_1 c_2 c_2' + 2 s_1 s_2 c_3 \Re(z) \\ (|z|\, s_2)^2 s_1 c_2 \\ (|z|\, s_1)^2 c_2 s_2 \\ (|z|\, s_1 s_2)^2 \end{pmatrix}. \tag{2.51}$$

In order to obtain an outer product representation for $\tilde{\rho}_{AB}^{GHZ}$, the following procedure is used. Firstly, find the spin flip of the orthonormal basis set given by Eq. (1.6) as

$$\begin{pmatrix} \text{Spin flip orthonormal} \\ \text{basis set for 2 qubits} \end{pmatrix} : \left\{ \left| \tilde{ij} \right\rangle \right\} \text{ for } i, j = 0, 1 \tag{2.52}$$

where

$$\left|\tilde{00}\right\rangle = \sigma_y^{\otimes 2} |00\rangle^* = (i\,|1\rangle)\,(i\,|1\rangle) = -\,|11\rangle\,, \tag{2.53}$$

$$\left|\tilde{01}\right\rangle = \sigma_y^{\otimes 2} |01\rangle^* = (i\,|1\rangle)\,(-i\,|0\rangle) = |10\rangle\,, \tag{2.54}$$

$$\left|\tilde{10}\right\rangle = \sigma_y^{\otimes 2} |10\rangle^* = (-i\,|0\rangle)\,(i\,|1\rangle) = |01\rangle\,, \tag{2.55}$$

$$\left|\tilde{11}\right\rangle = \sigma_y^{\otimes 2} |11\rangle^* = (-i\,|0\rangle)\,(-i\,|0\rangle) = -\,|00\rangle\,. \tag{2.56}$$

Secondly, use the spin flip states $|\,\tilde{\beta}_j\,\rangle = i \begin{pmatrix} -s_j \\ c_j \end{pmatrix}$ with $\left\langle 0 \middle| \tilde{\beta}_j \right\rangle = -i s_j$, $\left\langle 1 \middle| \tilde{\beta}_j \right\rangle = i c_j$, and $\left\langle \beta_j \middle| \tilde{\beta}_j \right\rangle = 0$

and the tensor product $|\,\tilde{\beta}_1\tilde{\beta}_2\,\rangle$ of the spin flip states $|\,\tilde{\beta}_j\,\rangle$ as

$$|\,\tilde{\beta}_1\tilde{\beta}_2\,\rangle = \begin{pmatrix} -s_1 s_2 \\ s_1 c_2 \\ c_1 s_2 \\ -c_1 c_2 \end{pmatrix} \tag{2.57}$$

with

$$\left\langle 00 \left|\tilde{\beta}_1\tilde{\beta}_2\right.\right\rangle = -s_1 s_2, \tag{2.58}$$

$$\left\langle 01 \left|\tilde{\beta}_1\tilde{\beta}_2\right.\right\rangle = s_1 c_2, \tag{2.59}$$

$$\left\langle 10 \left|\tilde{\beta}_1\tilde{\beta}_2\right.\right\rangle = c_1 s_2, \tag{2.60}$$

$$\left\langle 11 \left|\tilde{\beta}_1\tilde{\beta}_2\right.\right\rangle = -c_1 c_2 \tag{2.61}$$

as well as $\left\langle \beta_1\beta_2 \left|\tilde{\beta}_1\tilde{\beta}_2\right.\right\rangle = \left\langle \beta_1 \left|\tilde{\beta}_1\right.\right\rangle \left\langle \beta_2 \left|\tilde{\beta}_2\right.\right\rangle = 0$.

Finally, express spin flip states $|\tilde{a}_1\rangle$ and $|\tilde{a}_2\rangle$ using Eq. (2.43) as

$$|\tilde{a}_1\rangle = \frac{1}{N}\left(-|11\rangle + z^* c_3\,|\,\tilde{\beta}_1\tilde{\beta}_2\,\rangle\right) \tag{2.62}$$

and

$$|\tilde{a}_2\rangle = \frac{z^* s_3}{N}\,|\,\tilde{\beta}_1\tilde{\beta}_2\,\rangle\,. \tag{2.63}$$

All in all, start from Eq. (2.47) for ρ_{AB}^{GHZ}, then represent $\tilde{\rho}_{AB}^{GHZ}$ given by the Eq. (2.14) in the following form

$$\tilde{\rho}_{AB}^{GHZ} = |\tilde{a}_1\rangle\langle\tilde{a}_1| + |\tilde{a}_2\rangle\langle\tilde{a}_2| = \sum_{i=1}^{2} |\tilde{a}_i\rangle\langle\tilde{a}_i|\,. \tag{2.64}$$

A matrix representation of an operator $A : V \to W$, where V and W are any two vector spaces, is defined to be

$$A\left|v_j\right\rangle = \sum_i A_{ij}\,|w_i\rangle\,. \tag{2.65}$$

Here $\left\{\left|v_j\right\rangle\right\}$ and $\{|w_i\rangle\}$ are bases (not necessarily orthonormal) in spaces V and W respectively. The number of vectors in the basis set should be the same as the dimension of the corresponding vector space [36]. Also, A_{ij} are the matrix elements of the matrix representation of A. A_{ij} is the entry in the i^{th} row and the j^{th} column.

If $|a_1\rangle$ and $|a_2\rangle$ are the two elements of the basis set in V_{AB} (which is a four dimensional vector space since AB is a two qubit system) the rest of the basis set, say some mutually orthogonal states $|a_3\rangle$ and $|a_4\rangle$ can be chosen to be orthogonal to both $|\tilde{a}_1\rangle$ and $|\tilde{a}_2\rangle$, too, for convenience. Then, let $\rho_{AB}^{GHZ}\tilde{\rho}_{AB}^{GHZ}$ act on each element of the basis set $\left\{\left|a_j\right\rangle\right\}$ for $j = 1, 2, 3, 4$ to get

$$\rho_{AB}^{GHZ}\tilde{\rho}_{AB}^{GHZ}\left|a_j\right\rangle = \sum_{i=1}^{2}\left(AA^{\dagger}\right)_{ij}|a_i\rangle \tag{2.66}$$

where $A_{ik} = \langle a_i\,|\tilde{a}_k\,\rangle$. Therefore, $\rho_{AB}^{GHZ}\tilde{\rho}_{AB}^{GHZ}$ as an operator taking the vectors $\left\{\left|a_j\right\rangle\right\}$ from the vector space V_{AB} to the same vectors $\{|a_i\rangle\}$ in the four dimensional vector space V_{AB} represented by the 2×2 matrix $AA^{\dagger}$.

Now, use the calculated $\langle a_i | \tilde{a}_k \rangle$'s given below

$$\begin{aligned} \langle a_1 | \tilde{a}_1 \rangle &= -2\frac{z^*}{N^2} s_1 s_2 c_3, \\ \langle a_1 | \tilde{a}_2 \rangle &= -\frac{z^* s_1 s_2 s_3}{N^2} = \langle a_2 | \tilde{a}_1 \rangle, \\ \langle a_2 | \tilde{a}_2 \rangle &= 0 \end{aligned} \tag{2.67}$$

to get

$$A = \begin{pmatrix} \langle a_1 | \tilde{a}_1 \rangle & \langle a_1 | \tilde{a}_2 \rangle \\ \langle a_2 | \tilde{a}_1 \rangle & \langle a_2 | \tilde{a}_2 \rangle \end{pmatrix}. \tag{2.68}$$

Then $AA^\dagger$ is obtained as

$$AA^\dagger = \begin{pmatrix} |\langle a_1 | \tilde{a}_1 \rangle|^2 + |\langle a_1 | \tilde{a}_2 \rangle|^2 & \langle a_1 | \tilde{a}_1 \rangle \langle a_1 | \tilde{a}_2 \rangle^* \\ \langle a_1 | \tilde{a}_1 \rangle^* \langle a_1 | \tilde{a}_2 \rangle & |\langle a_1 | \tilde{a}_2 \rangle|^2 \end{pmatrix} \tag{2.69}$$

in terms of only $\langle a_i | \tilde{a}_k \rangle$'s for convenience.

Eigenvalues of $\rho_{AB}^{GHZ} \tilde{\rho}_{AB}^{GHZ}$ are the solution of the characteristic equation

$$c(\gamma) = \det\left(AA^\dagger - I\gamma\right) = 0 \tag{2.70}$$

with the solution

$$\gamma_1 = \frac{|z|^2 s_1^2 s_2^2}{N^4} (1 + c_3)^2 \text{ and } \gamma_2 = \frac{|z|^2 s_1^2 s_2^2}{N^4} (1 - c_3)^2. \tag{2.71}$$

Square roots of the eigenvalues γ_i found in Eq. (2.71) of $\rho_{AB}^{GHZ} \tilde{\rho}_{AB}^{GHZ}$ gives the set of eigenvalues λ_i of $R(\rho_{AB}^{GHZ})$ as

$$\{\lambda_1, \lambda_2, \lambda_3, \lambda_4\} = \left\{ \frac{|z| s_1 s_2}{N^2} (1 + c_3), \frac{|z| s_1 s_2}{N^2} (1 - c_3), 0, 0 \right\} \tag{2.72}$$

in non-increasing order. Using Eq. (2.16), the concurrence $C(\rho_{AB}^{GHZ})$ is finally calculated to be

$$C\left(\rho_{AB}^{GHZ}\right) = \frac{2 |z| s_1 s_2 c_3}{N^2} = |\langle a_1 | \tilde{a}_1 \rangle|. \tag{2.73}$$

CHAPTER 3

OPTIMAL ENSEMBLE REPRESENTING MIXED STATES

In this chapter, we can invoke what Kirkpatrick [55] call as Schrödinger-HJW theorem, a very useful result which has been discovered and re-discovered many times. It is first shown by Schrödinger in 1936 [40], later by Jaynes in 1957 [56], and by Hughston, Jozsa and Wootters in 1993 [57]. The theorem can be stated as follows: Suppose that we have an equality

$$\sum_{i=1}^{n} |\alpha_i\rangle \langle\alpha_i| = \sum_{j=1}^{m} \left|\beta_j\right\rangle \left\langle\beta_j\right| \tag{3.1}$$

where $|\alpha_1\rangle, \cdots, |\alpha_n\rangle, |\beta_1\rangle, \cdots, |\beta_m\rangle$ are some, possibly unnormalized vectors. The numbers n and m may be equal, but they may also be different. Suppose that $n \leq m$, without loss of generality. Then, there is an $m \times m$ unitary matrix U such that

$$|\alpha_i\rangle = \sum_{j=1}^{m} U_{ij} \,|\, \beta_j \,\rangle \qquad (\text{for } \; i = 1, 2, \cdots, n, n+1, \cdots, m)\,, \tag{3.2}$$

$$\left|\beta_j\right\rangle = \sum_{i=1}^{m} U^*_{ij} \,|\alpha_i\rangle \qquad (\text{for } \; j = 1, 2, \cdots, m) \tag{3.3}$$

where we define $|\alpha_{n+1}\rangle = |\alpha_{n+2}\rangle = \cdots = |\alpha_m\rangle = 0$.

It is straightforward to check that the opposite is also true, i.e., Eq. (3.2) [or Eq. (3.3)] implies Eq. (3.1). The proof of the actual theorem, i.e., Eq. (3.1) implies Eqs. (3.2) and (3.3), can be found in Nielsen [36] as well.

As in the discussion in Sec. 2.2, consider a mixed state $\rho = \rho_{AB}$ with matrix rank 2 so that it has only 2 non-zero eigenvalues. Therefore, we have

$$\rho_{AB} = \sum_{i=1}^{2} \beta_i \,|v_i\rangle \langle v_i| \tag{3.4}$$

where β_i are the eigenvalues corresponding to the mutually orthogonal eigenvectors $|v_i\rangle$ $(i = 1, 2)$.

In our case, consider any arbitrary ensemble $\mathscr{E} = \{r_i, |\, w_i\,\rangle\}$ with $n = 2$ states that realizes ρ_{AB}, then

$$\rho_{AB} = \sum_{i=1}^{2} \beta_i \,|v_i\rangle \langle v_i| = \sum_{i=1}^{2} r_i \,|w_i\rangle \langle w_i| \tag{3.5}$$

where r_i is the weight of the state $|\, w_i\,\rangle$ in the ensemble $\mathscr{E}$. Meanwhile, Eq. (3.5) can be expressed as

$$\rho_{AB} = \sum_{i=1}^{2} (|w_i\rangle \langle w_i|)_{sub} = \sum_{i=1}^{2} (|v_i\rangle \langle v_i|)_{sub}\,. \tag{3.6}$$

Here, the subscript *sub* stands for the *subnormalization* of $\mid v_i \rangle$ which is defined by

$$(\langle v_i \mid v_i \rangle)_{sub} = \beta_i \tag{3.7}$$

and also

$$(\langle w_i \mid w_i \rangle)_{sub} = r_i. \tag{3.8}$$

Therefore, by Schrödinger-HJW theorem we can find 2×2 unitary matrix U such that

$$|w_i\rangle_{sub} = \sum_{j=1}^{2} U_{ij}^{*} \left|v_j\right\rangle_{sub} \quad (for \quad i = 1, 2). \tag{3.9}$$

In this chapter, the main aim is to find the optimal ensemble[1]

$$\mathcal{E}^{opt} = \left\{p_i, |\psi_i\rangle_{AB}^{opt}\right\} \tag{3.10}$$

that represents ρ_{AB} for the matrix rank 2 states which are studied in chapter 2. This ensemble satisfies

$$\rho_{AB} = \sum_i p_i \left(|\psi_i\rangle \langle\psi_i|\right)_{AB}^{opt}. \tag{3.11}$$

Moreover, for this ensemble the average value of entanglement reaches its minimum value, i.e.,

$$E\left(C(\rho_{AB})\right) = \min \sum_i q_i E\left(\psi_{i,AB}\right) = \sum_i p_i E\left(\psi_{i,AB}^{opt}\right) \tag{3.12}$$

where $\{q_i, |\psi_i\rangle_{AB}\}$ is any ensemble having density matrix ρ_{AB} and the minimization is carried out over such ensembles. Here, $E\left(\psi_{i,AB}\right)$ is defined earlier as the von Neumann entropy by Eq. (2.2).

To find the optimal ensembles, only the types of density matrices for which $C(\rho) > 0$ are used since $C(\rho_{AB}^{W}) = 2\sqrt{x_1 x_2} > 0$ and $C\left(\rho_{AB}^{GHZ}\right) = 2\,|z|\, s_1 s_2 c_3/N^2 > 0$. For this type of density matrices, Wootters [54] proposes three successive decompositions of ρ_{AB} using *unitary* and *orthogonal transformations*. These decompositions are represented by the ensembles of $n = 2$ pure states which are listed as the following

$$\mathcal{E}(\rho_{AB}) = \begin{cases} \mathcal{E}_1 = \{r_i, \mid w_i \rangle\} \\ \mathcal{E}_2 = \{q_i, \mid y_i \rangle\} \\ \mathcal{E}_3 = \{h_i, \mid z_i \rangle\} \end{cases}. \tag{3.13}$$

The way to find these ensembles are described in the subsections of the following sections, in detail.

Briefly, in Sec. 3.1, the tool developed by Wootters [54] is utilized to obtain the optimal ensemble for mixed states with W class purifications. The set of states $\{\mid w_i \rangle\}$ in the first ensemble $\mathcal{E}_1$ are obtained by a unitary matrix U from the eigenvectors $\{\mid v_i \rangle\}$ using the Schrödinger-HJW theorem by Eq. (3.9). Then, the unitary matrix U is obtained easily so that it diagonalizes the matrix τ whose matrix elements are obtained by tilde-inner products defined by $\tau_{ij} = \left(\langle v_i \mid \tilde{v_j} \rangle\right)_{sub}$. By restricting $\mid w_i \rangle$ as

$$\left(\langle w_i \mid \tilde{w}_j \rangle\right)_{sub} = \lambda_i \delta_{ij} \tag{3.14}$$

where λ_i's are the eigenvalues of $R\left(\rho_{AB}^{W}\right)$ so that eigenvalues of $\tau\tau^*$ are equal to the absolute squares of λ_i.

[1] The superscript *opt* is the abbreviation of the word *optimal*.

Later, the set of states $\mid y_i \rangle$ in the second ensemble $\mathscr{E}_2$ are obtained from the set of states $\{\mid w_i \rangle\}$ in the previously determined ensemble $\mathscr{E}_1$. First, Wootters [54] defines the *preconcurrence* for any pure state $|\psi\rangle$ as follows

$$c(\psi) = \frac{\left(\langle \psi \mid \tilde{\psi} \rangle\right)_{sub}}{\left(\langle \psi \mid \psi \rangle\right)_{sub}}. \tag{3.15}$$

Next, the average preconcurrence of the ensemble $\mathscr{E}_2 = \{q_i, \mid y_i \rangle\}$ is chosen to be

$$\langle c(\mathscr{E}_2)\rangle = \sum_i q_i c(y_i) = \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4 = C(\rho_{AB}). \tag{3.16}$$

Here, $C(\rho_{AB})$ is the concurrence of the mixed state ρ_{AB}. Thus, Eq. (3.16) restricts the elements $\mid y_i \rangle$ to the relations

$$\mid y_1 \rangle_{sub} = \mid w_1 \rangle_{sub} \tag{3.17}$$

and

$$\mid y_j \rangle_{sub} = i \mid w_j \rangle_{sub} \qquad (for \quad j = 2, 3, 4) \tag{3.18}$$

because of the Eq. (3.14) for the elements $\mid w_i \rangle$. So, $\mid y_i \rangle$ is obtained from $\mid w_i \rangle$ easily.

The third ensemble $\mathscr{E}_3 = \{h_i, \mid z_i \rangle\}$, which will be our optimal ensemble, is obtained from the elements $\mid y_i \rangle$ of the second ensemble $\mathscr{E}_2$ using *real positive determinant orthogonal matrix* V. In this case, preconcurrences $c(z_i)$ of each state $\mid z_i \rangle$ in the ensemble are obtained by equating them to the average preconcurrence $\langle\, c(\mathscr{E}_3)\,\rangle$ of the ensemble $\mathscr{E}_3$, i.e., $C(\rho^W_{AB})$. This means that average entanglement $\sum_i h_i E(z_i)$ is equal to the entanglement $E\left(C(\rho^W_{AB})\right)$ of ρ^W_{AB} as given by Eq. (3.12).

However, in Sec. 3.2, a new approach is developed to do same for mixed states with GHZ class purifications. In this case, instead of finding the spectral decomposition of the ρ^{GHZ}_{AB}, the known decomposition $\rho^{GHZ}_{AB} = \sum_{i=1}^{2} |a_i\rangle\langle a_i|$ given by Eq. (2.47) is chosen to be the starting point. It is reasonable since finding the eigenvalues and eigenvectors of ρ^{GHZ}_{AB} is somewhat cumbersome. Therefore, the tilde inner product now is calculated by $\tau_{ij} = \langle\, a_i \mid \tilde{a}_j \,\rangle$. Now, construct the set of states $\{\mid w_i \rangle\}$ in the first ensemble $\mathscr{E}_1$ by the unitary matrix U from the set $\{|a_i\rangle\}$ using the Schrödinger-HJW theorem by Eq. (3.9), i.e., $\sqrt{r_i}\,|w_i\rangle = \sum_{j=1}^{2} U^*_{ij} \left|a_j\right\rangle$ for $(i = 1, 2)$. Then, the rest, i.e. determination of $\mid y_i \rangle$ and $\mid z_i \rangle$, is the same as the case of ρ^W_{AB}.

3.1 Mixed states with W class purifications

The eigenvalues β_i of ρ^W_{AB} are the roots of the characteristic equation

$$c(\gamma) \quad = \det\left(\rho^W_{AB} - \beta I\right) = \beta^2 \left\{\beta^2 - \beta + x_3(x_1 + x_2)\right\} \tag{3.19}$$

as

$$\{\beta_1, \beta_2, \beta_3, \beta_4\} \quad = \left\{\frac{1+\sqrt{\triangle}}{2}, \frac{1-\sqrt{\triangle}}{2}, 0, 0\right\} \tag{3.20}$$

where $\triangle = 1 - 4x_3(x_1 + x_2)$.

It is now sufficient to find the eigenvectors corresponding to the two nonzero eigenvalues β_1 and β_2 given by the Eq. (3.20). The solution to the eigenvector-eigenvalue relations $\rho^W_{AB}\,|v_i\rangle = \beta_i\,|v_i\rangle$ in terms of the entries of $|v_i\rangle$ is found to be

$$|v_i\rangle = \begin{pmatrix} a_i \\ b_i \\ c_i \\ d_i \end{pmatrix} = c_i \begin{pmatrix} \frac{1}{\sqrt{x_0 x_1}}\left(\beta_i - (x_1 + x_2)\right) \\ \sqrt{\frac{x_2}{x_1}} \\ 1 \\ 0 \end{pmatrix}. \tag{3.21}$$

It can be normalized for appropriate choice of c_i, but use the form given by the Eq. (3.21) for simplicity.

Subnormalization of $|v_i\rangle$ defined by the Eq. (3.7) is given by

$$(\langle\, v_i \,|\, v_i \,\rangle)_{sub} = \left\{ \frac{(\beta_i - x_1 - x_2)^2 + x_0 x_2}{x_0 x_1} + 1 \right\} c_i^2 = \beta_i \tag{3.22}$$

whose solution for c_i is

$$c_i = \sqrt{\frac{x_0 x_1 x_3}{(2\beta_i - 1)(\beta_i - 1 + x_3)}}. \tag{3.23}$$

Now, $|v_i\rangle$ is subnormalized if the value c_i found in Eq. (3.23) is put into Eq. (3.21) leading to $|v_i\rangle_{sub}$. It is convenient to leave these results with c_i given by Eq. (3.23) due to the reading convenience.

3.1.1 The first ensemble

Begin with the results of Eq. (3.9) obtained by Schrödinger-HJW theorem

$$|w_i\rangle_{sub} = \sum_{j=1}^{2} U_{ij}^* \left|v_j\right\rangle_{sub} \quad (\text{for } \; i = 1, 2) \tag{3.24}$$

for a 2×2 unitary matrix U. Therefore, the first ensemble $\mathscr{E}_1 = \{r_i, |\, w_i \,\rangle\}$ is obtained from the spectral decomposition of ρ_{AB}^W, i.e. $\{\beta_i, |v_i\rangle\}$. The subnormalized states $|v_i\rangle_{sub}$ are calculated by Eq. (3.21) where c_i is given by Eq. (3.23).

Now, define a 2×2 *symmetric,* but *not* necessarily Hermitian, matrix τ whose elements are constructed by *tilde inner products*

$$\tau_{ij} = \left(\langle\, v_i \,|\, \tilde{v_j} \,\rangle\right)_{sub}. \tag{3.25}$$

Here $|\, \tilde{v_j} \,\rangle_{sub}$ is the spin flip state $|\, v_j \,\rangle_{sub}$ defined by Eq. (2.9) such that

$$|\, \tilde{v_j} \,\rangle_{sub} = \sigma_y^{\otimes 2} \,|\, v_j^* \,\rangle_{sub}. \tag{3.26}$$

It is easy to show that the matrix τ defined by Eq. (3.25) is symmetric, i.e. $\tau_{ij} = \tau_{ji}$. Using Eq. (3.25) for $|\, \tilde{v_j} \,\rangle_{sub}$ we have

$$\begin{aligned}
\tau_{ij} &= \left(\langle\, v_i \,|\, \sigma_y^{\otimes 2} \,|\, v_j^* \,\rangle\right)_{sub} = \left(\langle\, v_j^* \,|\, \left(\sigma_y^{\otimes 2}\right)^\dagger \,|\, v_i \,\rangle\right)_{sub}^* \\
&= \left(\langle\, v_j^* \,|\, \sigma_y^{\otimes 2} \,|\, v_i \,\rangle\right)_{sub}^* = \left(\langle\, v_j^* \,|\, \tilde{v_i}^* \,\rangle\right)_{sub}^* \\
&= \left(\langle\, v_j \,|\, \tilde{v_i} \,\rangle^*\right)_{sub}^* = \left(\langle\, v_j \,|\, \tilde{v_i} \,\rangle\right)_{sub} = \tau_{ji}
\end{aligned} \tag{3.27}$$

because $\sigma_y^{\otimes 2}$ is Hermitian and real by Eq. (2.31). As a result, τ is a symmetric matrix. However, it is not necessarily Hermitian since

$$\left(\tau^\dagger\right)_{ij} = \tau_{ji}^* = \left(\langle\, v_j \,|\, \tilde{v_i} \,\rangle\right)_{sub}^* = \left(\langle\, \tilde{v_i} \,|\, v_j \,\rangle\right)_{sub} \neq \tau_{ij}. \tag{3.28}$$

For the set $\{\lambda_i\}$ of the non-negative eigenvalues Eq. (2.36) of the *R matrix,* $R(\rho_{AB}^W)$, let $|w_i\rangle_{sub}$ be given by Eq. (3.24). It satisfies the condition $\left(\langle\, w_i \,|\, \tilde{w}_j \,\rangle\right)_{sub} = \lambda_i \delta_{ij}$ as previously assumed by Eq. (3.14) where the spin flip state $|\, \tilde{w}_i \,\rangle_{sub}$ is

$$|\, \tilde{w}_i \,\rangle_{sub} = \sigma_y^{\otimes 2} \,|\, w_i^* \,\rangle_{sub} = \sum_{j=1}^{2} U_{ij} \,|\, \tilde{v_j} \,\rangle_{sub}. \tag{3.29}$$

Then, Eq. (3.14) can also be written in terms of U and τ as the following

$$\begin{aligned}\langle\, w_i \mid \tilde{w}_j \,\rangle_{sub} &= \sum_{k,l=1}^{2} U_{ik}U_{jl}\langle\, v_k \mid \tilde{v}_l \,\rangle_{sub} = \sum_{k,l=1}^{2} U_{ik}\tau_{kl}U^T_{lj} \\ &= \left(U\tau U^T\right)_{ij} = \lambda_i\delta_{ij}. \end{aligned} \tag{3.30}$$

Eq. (3.30) implies that $U\tau U^T$ is diagonal with the diagonal elements λ_i and there is a unitary U that diagonalizes τ. However, the diagonalization of $\tau\tau^*$ gives us a wider aspect. First, multiply $U\tau U^T$ with $\left(U\tau U^T\right)^* = U^*\tau^*U^\dagger$ to obtain

$$\begin{aligned}\left\{U\tau U^T U^*\tau^*U^\dagger\right\}_{ij} &= \left\{U\tau\left(U^\dagger U\right)^*\tau^*U^\dagger\right\}_{ij} = \left(U\tau\tau^*U^\dagger\right)_{ij} \\ &= \sum_k \left(U\tau U^T\right)_{ik}\left(U^*\tau^*U^\dagger\right)_{kj} \\ &= |\lambda_i|^2\,\delta_{ij} \end{aligned} \tag{3.31}$$

so

$$\left(U\tau\tau^*U^\dagger\right)_{ij} = |\lambda_i|^2 = \lambda_i^2 \tag{3.32}$$

since $\lambda_1 = 2\sqrt{x_1x_2}$ and $\lambda_2 = 0$ are real.

Thus, in general, we deduce that $\tau\tau^*$ is Hermitian because it is diagonalized by the unitary matrix U and its eigenvalues are the absolute squares of the eigenvalues of the matrix $R(\rho^W_{AB})$. This means that $\tau\tau^*$ has a spectral spectral decomposition

$$\tau\tau^* = \sum_{i=1}^{2}\lambda_i^2\,|t_i\rangle\langle t_i| \tag{3.33}$$

if $|t_i\rangle$'s are the orthonormal eigenvectors of $\tau\tau^*$ corresponding to the eigenvalues λ_i^2.

Using the results above, we claim that the rows (or the columns) of a unitary U (or $U^\dagger$) that diagonalizes $\tau\tau^*$ can be chosen as the eigenbras (or the eigenkets) of $\tau\tau^*$ in the proper order of the eigenvectors corresponding to the eigenvalues λ_i^2 as the following

$$U^\dagger = \begin{pmatrix} |t_1\rangle & |t_2\rangle \end{pmatrix}. \tag{3.34}$$

So U satisfies the completeness equation $U^\dagger U = UU^\dagger = I$. Indeed, U diagonalizes $\tau\tau^*$ to its spectral form as the following

$$U\tau\tau^*U^\dagger = \begin{pmatrix} \langle t_1| \\ \langle t_2| \end{pmatrix}(\tau\tau^*)\begin{pmatrix} |t_1\rangle & |t_2\rangle \end{pmatrix} = \begin{pmatrix} \lambda_1^2 & 0 \\ 0 & \lambda_2^2 \end{pmatrix} \tag{3.35}$$

where we used Eq. (3.33) to have $\tau\tau^*\,|t_i\rangle = \lambda_i^2\,|t_i\rangle$.

Now, we find the elements τ_{ij} by Eq. (3.25) for $|\, v_i \,\rangle_{sub}$'s in terms of the coefficients c_i by Eq. (3.23) and we get

$$\tau_{ij} = \langle\, v_i \mid \tilde{v}_j \,\rangle_{sub} = 2\left(\sqrt{\frac{x_2}{x_1}}\right)c_ic_j. \tag{3.36}$$

Next, construct the matrix elements $(\tau\tau^*)_{ij}$ of $\tau\tau^*$ as

$$(\tau\tau^*)_{ij} = \sum_{k=1}^{2}\tau_{ik}\tau^*_{kj} = \left(\frac{4x_2}{x_1}\right)\left(c_ic_j\right)\sum_{k=1}^{2}c_k^2. \tag{3.37}$$

After detailed calculations, we find the following expression $\sum_{k=1}^{2} c_k^2 = x_1$ and get $(\tau\tau^*)_{ij} = 4x_2 c_i c_j$ such that

$$\tau\tau^* = 4x_2 \begin{pmatrix} c_1^2 & c_1 c_2 \\ c_1 c_2 & c_2^2 \end{pmatrix} \tag{3.38}$$

which is a Hermitian matrix as proved in Eq. (3.33).

Using the fact that $\tau\tau^*$ has only one-nonzero eigenvalue $\lambda_1^2 = 4x_1 x_2$ with the others being $\lambda_{2,3,4} = 0$, the eigenvector of $\tau\tau^*$ corresponding to the eigenvalue λ_1^2 can be found as

$$|\, t_1 \,\rangle = \frac{1}{\sqrt{x_1}} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} .$$

The second eigenvector corresponding to the eigenvalue $\lambda_2^2 = 0$ will be orthogonal to $|\, t_1 \,\rangle$. Therefore, we obtain

$$|\, t_2 \,\rangle = \frac{1}{\sqrt{x_1}} \begin{pmatrix} c_2 \\ -c_1 \end{pmatrix} ,$$

an therefore the unitary matrix U is

$$U = \begin{pmatrix} \langle t_1| \\ \langle t_2| \end{pmatrix} = \frac{1}{\sqrt{x_1}} \begin{pmatrix} c_1 & c_2 \\ c_2 & -c_1 \end{pmatrix}. \tag{3.39}$$

As a result, using Eq. (3.39) for U, then $|\, w_1 \,\rangle_{sub}$ of the first decomposition $\mathscr{E}_1$ is calculated as

$$\begin{aligned} |\, w_1 \,\rangle_{sub} &= \sum_{j=1}^{2} U_{1j}^* |\, v_j \,\rangle_{sub} \\ &= \left(\frac{c_1}{\sqrt{x_1}}\right) |\, v_1 \,\rangle_{sub} + \left(\frac{c_2}{\sqrt{x_1}}\right) |\, v_2 \,\rangle_{sub} . \end{aligned} \tag{3.40}$$

After detailed calculations, we get

$$|\, w_1 \,\rangle_{sub} = \sqrt{x_0}\,|00\rangle + \sqrt{x_2}\,|01\rangle + \sqrt{x_1}\,|10\rangle . \tag{3.41}$$

Therefore, putting Eq. (3.41) into the subnormalization formula for $|\, w_1 \,\rangle$ by Eq. (3.8), we find the probability r_1 to obtain $|\, w_1 \,\rangle$ in the ensemble $\mathscr{E}_1 = \{r_i, |\, w_i \,\rangle\}$ as

$$\langle\, w_1 \,|\, w_1 \,\rangle_{sub} = r_1 = x_0 + x_1 + x_2 = 1 - x_3 \tag{3.42}$$

and $|\, w_1 \,\rangle$ is found to be

$$\begin{aligned} |\, w_1 \,\rangle &= \frac{1}{\sqrt{r_1}} |\, w_1 \,\rangle_{sub} \\ &= \frac{1}{\sqrt{1 - x_3}} \left(\sqrt{x_0}\,|00\rangle + \sqrt{x_2}\,|01\rangle + \sqrt{x_1}\,|10\rangle \right). \end{aligned} \tag{3.43}$$

Next, to find the second member $|\, w_2 \,\rangle$ of the ensemble $\mathscr{E}_1$, use the preceding procedure to get

$$\begin{aligned} |\, w_2 \,\rangle_{sub} &= \sum_{j=1}^{2} U_{2j}^* |\, v_j \,\rangle_{sub} \\ &= \left(\frac{c_2}{\sqrt{x_1}}\right) |\, v_1 \,\rangle_{sub} - \left(\frac{c_1}{\sqrt{x_1}}\right) |\, v_2 \,\rangle_{sub} && (3.44) \\ &= \sqrt{x_3}\,|00\rangle && (3.45) \end{aligned}$$

and by Eq. (3.8), we find the probability r_2 for $|\, w_2 \,\rangle$ in the ensemble $\mathscr{E}_1$ as

$$\langle\, w_2 \,|\, w_2 \,\rangle_{sub} = r_2 = x_3. \tag{3.46}$$

Finally $|\, w_2 \,\rangle$ is found to be

$$|\, w_2 \,\rangle \equiv \frac{1}{\sqrt{x_3}} |\, w_2 \,\rangle_{sub} = |00\rangle\,. \tag{3.47}$$

For consistency, note that the sum of probabilities $\{r_1, r_2\}$ found in Eqs. (3.42) and (3.46) is 1, i.e., $r_1 + r_2 = 1 - x_3 + x_3 = 1$.

3.1.2 The second ensemble

The set of states $|\, y_i \,\rangle$ in the second ensemble $\mathscr{E}_2 = \{q_i, |\, y_i \,\rangle\}$ $(i = 1, 2)$ are obtained from the first ensemble $\mathscr{E}_1 = \{r_i, |\, w_i \,\rangle\}$ found in Sec. 3.1.1 so that

$$\sum_{i=1}^{2} (|\, y_i \,\rangle\langle\, y_i \,|)_{sub} = \sum_{i=1}^{2} (|\, w_i \,\rangle\langle\, w_i \,|)_{sub} = \rho^{W}_{AB} \tag{3.48}$$

where $|\, y_i \,\rangle_{sub} = \sqrt{q_i}\,|\, y_i \,\rangle$.

Using the preconcurrence formula given by Eq. (3.15) for $|\, y_i \,\rangle$, we get

$$c\,(y_i) = \frac{(\langle\, y_i \,|\, \tilde{y}_i \,\rangle)_{sub}}{(\langle\, y_i \,|\, y_i \,\rangle)_{sub}} = \frac{(\langle\, y_i \,|\, \tilde{y}_i \,\rangle)_{sub}}{q_i}. \tag{3.49}$$

Next, the average preconcurrence of the ensemble $\mathscr{E}_2 = \{q_i, |\, y_i \,\rangle\}$ is chosen to be equal to

$$\langle c\,(\mathscr{E}_2)\rangle = \sum_{i=}^{2} q_i c\,(y_i) = \lambda_1 - \lambda_2 = 2\sqrt{x_1 x_2} = C\,(\rho_{AB})\,. \tag{3.50}$$

Here, $C\,(\rho_{AB})$ is the concurrence of the mixed state ρ^{W}_{AB}. Thus, Eq. (3.50) restricts the elements $|\, y_i \,\rangle$ to such relations

$$|\, y_1 \,\rangle_{sub} = |\, w_1 \,\rangle_{sub} \tag{3.51}$$

and

$$|\, y_2 \,\rangle_{sub} = i\,|\, w_2 \,\rangle_{sub} \tag{3.52}$$

since $\left(\langle\, w_i \,|\, \tilde{w}_j \,\rangle\right)_{sub} = \lambda_i \delta_{ij}$ by Eq. (3.14). Therefore, $\mathscr{E}_2$ satisfies $\langle c\,(\mathscr{E}_2)\rangle = C\,(\rho_{AB})$ given by Eq. (3.50) such that

$$\begin{aligned}
\langle c\,(\mathscr{E}_2)\rangle &= (\langle\, y_1 \,|\, \tilde{y}_1 \,\rangle)_{sub} + (\langle\, y_2 \,|\, \tilde{y}_2 \,\rangle)_{sub} \\
&= (\langle\, w_1 \,|\, \tilde{w}_1 \,\rangle)_{sub} - (\langle\, w_2 \,|\, \tilde{w}_2 \,\rangle)_{sub} \\
&= \lambda_1 - \lambda_2 = 2\sqrt{x_1 x_2} = C\,(\rho_{AB})\,.
\end{aligned} \tag{3.53}$$

Now, we derive the elements $\{|\, y_i \,\rangle\}_{i=1,2}$ of the second decomposition $\mathscr{E}_2 = \{q_i, |\, y_i \,\rangle\}$ realizing ρ^{W}_{AB} from the first ensemble $\mathscr{E}_1 = \{r_i, |\, w_i \,\rangle\}$ obtained is the Sec.(3.1.1) as

$$\begin{aligned}
|\, y_1 \,\rangle_{sub} &= \sqrt{q_1}\,|\, y_1 \,\rangle = |\, w_1 \,\rangle_{sub} \\
&= \sqrt{x_0}\,|00\rangle + \sqrt{x_2}\,|01\rangle + \sqrt{x_1}\,|10\rangle\,,
\end{aligned} \tag{3.54}$$

then

$$|\, y_1 \,\rangle = \frac{1}{\sqrt{1 - x_3}} \left(\sqrt{x_0}\,|00\rangle + \sqrt{x_2}\,|01\rangle + \sqrt{x_1}\,|10\rangle\right) \tag{3.55}$$

and

$$| y_2 \rangle_{sub} = \sqrt{q_2} | y_2 \rangle = i | w_2 \rangle_{sub} = i \sqrt{x_3} |00\rangle \tag{3.56}$$

then

$$| y_2 \rangle = \frac{1}{\sqrt{q_2}} | y_2 \rangle_{sub} = i |00\rangle . \tag{3.57}$$

Note that the probabilities q_i of $| y_i \rangle$ in the ensemble $\mathscr{E}_2$ are equal to the probabilities of r_i of $| w_i \rangle$ in the ensemble $\mathscr{E}_1$ given by , i.e. $q_1 = r_1 = 1 - x_3$ and $q_2 = r_2 = x_3$.

3.1.3 The optimal ensemble

3.1.3.1 Prescription

Compared to the other first two ensembles $\mathscr{E}_1$ and $\mathscr{E}_2$ discussed in the previous sections, now let the last ensemble, $\mathscr{E}_3 = \{h_i, | z_i \rangle\}$, be the optimal ensemble as Wootters proposes [54]. This decomposition is arranged in such a way that preconcurrences $c(z_i)$ of each states $| z_i \rangle$ in the ensemble are equal to the average preconcurrence $\langle c(\mathscr{E}_3) \rangle$ of the ensemble $\mathscr{E}_3$ which is equal to $C(\rho^W_{AB})$. Accordingly, entanglement $E(z_i)$ of each states $| z_i \rangle$ in the ensemble will be equal to the average entanglement $\langle E(\mathscr{E}_3) \rangle = \sum_{i=1}^{2} h_i E(z_i)$ of the ensemble which is equal to $E(C(\rho_{AB}))$.

Now, we make use of the formula for the first ensemble $\mathscr{E}_1$ given by Eq. (3.9) of ρ^W_{AB} so that

$$| z_i \rangle_{sub} = \sum_{j=1}^{2} V^*_{ij} | y_j \rangle_{sub} \tag{3.58}$$

for a 2×2 unitary matrix V.

For further discussions, Wootters [54] defines a 2×2 matrix Y whose elements are given by

$$Y_{ij} = \langle y_i | \tilde{y}_j \rangle_{sub} \tag{3.59}$$

which are found to be

$$Y_{11} = \langle y_1 | \tilde{y_1} \rangle_{sub} = 2 \sqrt{x_1 x_2} \tag{3.60}$$

with the other elements being zero. Consequently, written in a matrix form, Y becomes

$$Y = \begin{pmatrix} 2\sqrt{x_1 x_2} & 0 \\ 0 & 0 \end{pmatrix} \tag{3.61}$$

which is a *real diagonal* matrix.

Thus, the average preconcurrence is

$$\langle c(\mathscr{E}_3) \rangle = \sum_{i=1}^{2} h_i c(z_i) = \sum_{i=1}^{2} \langle z_i | \tilde{z}_i \rangle_{sub} \tag{3.62}$$

$$= \sum_{i=1}^{2} \sum_{k,l=1}^{2} V_{ik} Y_{kl} V^T_{li} = \sum_{i=1}^{2} \left(VYV^T \right)_{ii}$$

$$= \mathrm{tr}\left(VYV^T \right) . \tag{3.63}$$

In this decomposition, let the unitary matrix V be also a real matrix, that is, it is an orthogonal matrix with the property $V^\dagger = V^T \Rightarrow V^T V = I \Rightarrow V^T = V^{-1}$. In such a case, the average preconcurrence $\langle\, c(\mathscr{E}_3)\,\rangle$ remains invariant under transformations by the 2×2 real orthogonal matrices. Since the trace of Y is preserved due to the cyclic property of the trace operation, $\mathrm{tr}(ABC) = \mathrm{tr}(BCA) = \mathrm{tr}(CAB)$, then

$$\begin{aligned}\langle\, c(\mathscr{E}_3)\,\rangle &= \mathrm{tr}\left(VYV^T\right) = \mathrm{tr}\left(VYV^{-1}\right)\\ &= \mathrm{tr}\left(V^{-1}VY\right) = \mathrm{tr}Y = 2\sqrt{x_1x_2} = C(\rho^W_{AB}).\end{aligned} \tag{3.64}$$

Put it in another way, the last decomposition $\mathscr{E}_3 = \{h_i, |\, z_i\,\rangle\}$ derived by the orthogonal transformations of $\{|\, y_i\,\rangle\}$ is the optimal ensemble $\mathscr{E}^{opt}$. However, as described in the paragraph above, we are interested only in the transformation that makes the individual preconcurrences $c(z_i)$ equal to the average preconcurrence $\langle\, c(\mathscr{E}_3)\,\rangle$ of the ensemble.

3.1.3.2 Orthogonal matrix V

As discussed in the previous section, the preconcurrence of $|\, z_1\,\rangle$ must be equal to $C(\rho^W_{AB})$ such that

$$c(z_1) = \frac{\langle\, z_1 \,|\, \tilde{z}_1\,\rangle_{sub}}{\langle\, z_1\,|\, z_1\,\rangle_{sub}} = \frac{\left(VYV^T\right)_{11}}{h_1} = 2\sqrt{x_1x_2} \tag{3.65}$$

and of $|\, z_2\,\rangle$:

$$c(z_2) = \frac{\langle\, z_2 \,|\, \tilde{z}_2\,\rangle}{\langle\, z_2\,|\, z_2\,\rangle} = \frac{\left(VYV^T\right)_{22}}{h_2} = 2\sqrt{x_1x_2}. \tag{3.66}$$

Next, consider a real orthogonal matrix V with a positive determinant. The columns and rows of V form orthonormal sets. Then, in order to obtain a positive determinant for V, i.e.,

$$\det(V) = V_{11}V_{22} - V_{12}V_{21} > 0, \tag{3.67}$$

the following matrix can be obtained

$$V = \begin{pmatrix} \sqrt{h_1} & -\sqrt{h_2} \\ \sqrt{h_2} & \sqrt{h_1} \end{pmatrix}. \tag{3.68}$$

3.1.3.3 The third ensemble

Ultimately, one can construct the set of states $\{|\, z_i\,\rangle\}$ in the third ensemble $\mathscr{E}_3 = \{h_i, |\, z_i\,\rangle\}$ from the set of states $\{|\, y_i\,\rangle\}$ in the second ensemble $\mathscr{E}_2 = \{q_i, |\, y_i\,\rangle\}$ by the orthogonal matrix V given by Eq. (3.68). We use Eq. (3.58) to get

$$\begin{aligned}|\, z_1\,\rangle_{sub} &= V^*_{11}\,|\, y_1\,\rangle_{sub} + V^*_{12}\,|\, y_2\,\rangle_{sub}\\ &= \left(\sqrt{h_1x_0} - i\sqrt{h_2x_3}\right)|00\rangle\\ &+\sqrt{h_1}\left(\sqrt{x_2}\,|01\rangle + \sqrt{x_1}\,|10\rangle\right)\end{aligned} \tag{3.69}$$

and

$$|\, z_2\,\rangle_{sub} = \left(\sqrt{h_2x_0} + i\sqrt{h_1x_3}\right)|00\rangle + \sqrt{h_2}\left(\sqrt{x_2}\,|01\rangle + \sqrt{x_1}\,|10\rangle\right). \tag{3.70}$$

Finally optimal states which are equal to $\{|\ z_i\ \rangle\}$ become

$$\left|\psi_1^{opt}\right\rangle_{AB} = \left(\sqrt{x_0} - i\sqrt{\frac{p_2 x_3}{p_1}}\right)|00\rangle + \sqrt{x_2}\,|01\rangle + \sqrt{x_1}\,|10\rangle \tag{3.71}$$

with probability p_1 and

$$\left|\psi_2^{opt}\right\rangle_{AB} = \left(\sqrt{x_0} + i\sqrt{\frac{p_1 x_3}{p_2}}\right)|00\rangle + \sqrt{x_2}\,|01\rangle + \sqrt{x_1}\,|10\rangle \tag{3.72}$$

with probability p_2 for being in the optimal ensemble $\mathscr{E}^{opt} = \left\{p_i, |\ \psi_i^{opt}\ \rangle_{AB}\right\}$. However, by normalization of $|\ \psi_i^{opt}\ \rangle_{AB}$ and the equation $\sum_{m=0}^{3} x_m = 1$, the values of p_i's are obtained easily as

$$p_1 = p_2 = \frac{1}{2}. \tag{3.73}$$

Therefore, the following results are obtained

$$V = \begin{pmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{pmatrix}, \tag{3.74}$$

$$\left|\psi_1^{opt}\right\rangle_{AB} = \left(\sqrt{x_0} - i\sqrt{x_3}\right)|00\rangle + \sqrt{x_2}\,|01\rangle + \sqrt{x_1}\,|10\rangle\,, \tag{3.75}$$

and

$$\left|\psi_2^{opt}\right\rangle_{AB} = \left(\sqrt{x_0} + i\sqrt{x_3}\right)|00\rangle + \sqrt{x_2}\,|01\rangle + \sqrt{x_1}\,|10\rangle\,. \tag{3.76}$$

3.2 Mixed states with GHZ class purifications

In this section, we use the same procedure prescribed by Wootters [(54)] to find the optimal ensemble representing ρ_{AB}^{GHZ}. However, as shown in the Appendix A, the eigenvalues and eigenvectors of ρ_{AB}^{GHZ} are not manipulated easily like in the case of ρ_{AB}^{W} (See Sec. 3.1). Then, we claim that since we have an available ensemble representing ρ_{AB}^{GHZ}, i.e., $\rho_{AB}^{GHZ} = \sum_{i=1}^{2} |a_i\rangle\langle a_i|$ which is given by Eq. (2.47), then it is better to start with this ensemble. In this case, there is no loss in generality. In other words, it is unnecessary to start with the spectral decomposition of ρ_{AB}^{GHZ} in order to obtain the optimal ensemble. The following sections describe this new method.

3.2.1 The first ensemble

Looking from the ensemble picture defined by Eq. (1.8), there is an ensemble

$$\mathscr{E}_a = \left\{a_i, \left|a_i'\right\rangle\right\} \tag{3.77}$$

realizing ρ_{AB}^{GHZ} given by Eq. (2.47). Namely,

$$\rho_{AB}^{GHZ} = \sum_{i=1}^{2} |a_i\rangle\langle a_i| = \sum_{i=1}^{2} p_i \left|a_i'\right\rangle\left\langle a_i'\right| \tag{3.78}$$

for the already *subnormalized states* $|a_i\rangle = \sqrt{a_i}\left|a_i'\right\rangle$ with the probability a_i being the square of norm of $|a_i\rangle$.

We argue that the set of states $\{|w_i\rangle\}$ in the first ensemble $\mathscr{E}_1 = \{r_i, |w_i\rangle\}$ defined by Eq. (3.9) can directly be obtained by the set of states $\{|a_i\rangle\}$ in the ensemble $\mathscr{E}_a = \left\{a_i, \left|a_i'\right\rangle\right\}$ given by Eq. (3.77). This is to say that there is a unitary matrix U between the states $\{|w_i\rangle\}$ and $\{|a_i\rangle\}$ with the following relation

$$|w_i\rangle_{sub} = \sum_{j=1}^{2} U_{ij}^{*} \left|a_j\right\rangle \quad for \quad i = 1, 2 \tag{3.79}$$

where $|w_i\rangle_{sub} = \sqrt{r_i}\,|w_i\rangle$. Following the procedure used in the previous section, there is a constraint defined by Eq. (3.14) on the set of states $\{|w_i\rangle\}$ such that

$$\left(\left\langle w_i \middle| \tilde{w}_j \right\rangle\right)_{sub} = \lambda_i \delta_{ij}. \tag{3.80}$$

Here, $\{\lambda_i\}$ is the set of eigenvalues of the matrix $R\left(\rho_{AB}^{GHZ}\right)$ given by Eq. (2.72). Hence, the elements of the matrix τ is obtained by the tilde inner product by

$$\tau_{ij} = \left\langle a_i \middle| \tilde{a}_j \right\rangle \tag{3.81}$$

so that

$$U\tau\tau^{*}U^{\dagger} = \lambda_i^2 \delta_{ij}. \tag{3.82}$$

We will then find the unitary matrix with $U = \begin{pmatrix} \langle t_1| \\ \langle t_2| \end{pmatrix}$ which diagonalizes the matrix $\tau\tau^{*}$. Remember that $|t_i\rangle$ is the eigenvector of $\tau\tau^{*}$ corresponding to the eigenvalue λ_i^2.

Now, we use the values of $\left\langle a_i \middle| \tilde{a}_j \right\rangle$'s which are given by Eq. (2.67) which are τ_{ij}'s defined by Eq. (3.81). Therefore, we have

$$\tau = \begin{pmatrix} \langle a_1 | \tilde{a}_1 \rangle & \langle a_1 | \tilde{a}_2 \rangle \\ \langle a_2 | \tilde{a}_1 \rangle & 0 \end{pmatrix} = \frac{\langle a_1 | \tilde{a}_1 \rangle}{2c_3} \begin{pmatrix} 2c_3 & s_3 \\ s_3 & 0 \end{pmatrix} \tag{3.83}$$

since

$$\frac{\langle a_1 | \tilde{a}_2 \rangle}{\langle a_1 | \tilde{a}_1 \rangle} = \frac{-z^{*} s_1 s_2 s_3 \big/ N^2}{-2z^{*} s_1 s_2 c_3 \big/ N^2} = \frac{s_3}{2c_3}. \tag{3.84}$$

Notice that τ found in Eq. (3.83) is a real Hermitian matrix

$$H = \begin{pmatrix} 2c_3 & s_3 \\ s_3 & 0 \end{pmatrix} \tag{3.85}$$

multiplied by a complex number $\langle a_1 | \tilde{a}_1 \rangle / 2c_3$. In other words, τ^{*} is also the same Hermitian matrix multiplied by $\langle a_1 | \tilde{a}_1 \rangle^{*} / 2c_3$. Then, it is straightforward to show that $\tau\tau^{*}$ has the same eigenvectors as those of H. If calculated, the eigenvalues of H are found to be $\alpha_{1,2} = c_3 \pm 1$. Thus, the eigenvectors of H are obtained as

$$|t_1\rangle = \frac{1}{\sqrt{2(1-c_3)}} \begin{pmatrix} 1-c_3 \\ s_3 \end{pmatrix}, \quad |t_2\rangle = \frac{1}{\sqrt{2(1-c_3)}} \begin{pmatrix} s_3 \\ c_3-1 \end{pmatrix} \tag{3.86}$$

corresponding to the eigenvalues $\alpha_{1,2}$ respectively.

Consequently, the unitary matrix U can be expressed as

$$U = \frac{1}{\sqrt{2(1-c_3)}} \begin{pmatrix} 1-c_3 & s_3 \\ s_3 & c_3-1 \end{pmatrix} \tag{3.87}$$

which is also a real Hermitian matrix. Hence, by the Eq. (3.79), the subnormalized forms of the states $|w_i\rangle$ of the first ensemble $\mathscr{E}_1$ are obtained from the states $\{|a_i\rangle\}$ in the ensemble $\mathscr{E}_a$ as

$$|w_1\rangle_{sub} = \frac{1}{\sqrt{2(1-c_3)}} \{(1-c_3)|a_1\rangle + s_3 |a_2\rangle\} \tag{3.88}$$

and

$$|w_2\rangle_{sub} = \frac{1}{\sqrt{2(1-c_3)}} \{s_3 |a_1\rangle + (c_3 - 1)|a_2\rangle\}. \tag{3.89}$$

It can be shown that the probability r_i of $|w_i\rangle$ in the ensemble $\mathscr{E}_1 = \{r_i, |w_i\rangle\}$ is equal to the probability a_i of $\left|a'_i\right\rangle$ in $\mathscr{E}_a = \left\{a_i, \left|a'_i\right\rangle\right\}$ so that

$$r_1 = a_1 = \||a_1\rangle\|^2 = \frac{N^2 - s_3^2 |z|^2}{N^2}, \quad r_2 = \||a_2\rangle\|^2 = \frac{s_3^2 |z|^2}{N^2} \tag{3.90}$$

where $\{|a_i\rangle\}$ are defined by Eq. (2.43). Finally, by definition $|w_i\rangle_{sub} = \sqrt{r_i}\, |w_i\rangle$ and substituting the open forms of $\{|a_i\rangle\}$ given by Eq. (2.43) into the result, we have

$$|w_1\rangle = \kappa_1 \left\{|00\rangle + z\left(c_3 + \frac{s_3^2}{1-c_3}\right)|\beta_1\beta_2\rangle\right\} \tag{3.91}$$

and

$$|w_2\rangle = \kappa_2 \{|00\rangle + z(2c_3 - 1)|\beta_1\beta_2\rangle\} \tag{3.92}$$

where

$$\kappa_1 = \sqrt{\frac{1-c_3}{2\left(N^2 - s_3^2 |z|^2\right)}}, \quad \kappa_2 = \sqrt{\frac{1}{2|z|(1-c_3)}}. \tag{3.93}$$

3.2.2 The second ensemble

Similar discussions with the case of W class applies here to obtain the second ensemble $\mathscr{E}_2 = \{q_i, |\, y_i\, \rangle\}$ $(i = 1, 2)$ from the first ensemble $\mathscr{E}_1 = \{r_i, |\, w_i\, \rangle\}$ found in Sec. 3.2.1. Therefore,

$$|y_1\rangle = |w_1\rangle = \kappa_1 \left\{|00\rangle + z\left(c_3 + \frac{s_3^2}{1-c_3}\right)|\beta_1\beta_2\rangle\right\} \tag{3.94}$$

and

$$|y_2\rangle = i\,|w_2\rangle = i\kappa_2 \{|00\rangle + z(2c_3 - 1)|\beta_1\beta_2\rangle\} \tag{3.95}$$

where κ_1 and κ_2 are given by Eq. (3.93). Also, since $|y_i\rangle_{sub} = \sqrt{q_i}\, |y_i\rangle$ and

$$\||y_i\rangle\|_{sub} = \||w_i\rangle\|_{sub}, \tag{3.96}$$

then the probabilities q_i of $|y_i\rangle$ in $\mathscr{E}_2$ are the same as the probabilities r_i of $|w_i\rangle$ in $\mathscr{E}_1$, namely

$$q_1 = r_1 = \frac{N^2 - s_3^2 |z|^2}{N^2}, \quad q_2 = r_2 = \frac{s_3^2 |z|^2}{N^2}. \tag{3.97}$$

3.2.3 The optimal ensemble

As summarized in Sec. 3.1.3 for the W case, we now find a real diagonal 2×2 matrix Y whose diagonal elements are obtained by the Eq. (3.59) so that

$$Y = \begin{pmatrix} \lambda_1 & 0 \\ 0 & -\lambda_2 \end{pmatrix}. \tag{3.98}$$

Here, λ_i's are the eigenvalues of the matrix $R\left(\rho_{AB}^{GHZ}\right)$ in non-increasing order given by the Eq. (2.72). Note that

$$\mathrm{tr}Y = \lambda_1 - \lambda_2 = C\left(\rho_{AB}^{GHZ}\right) \tag{3.99}$$

as also proved by Eq (3.64).

Now, in order for each preconcurrence of the states $|z_i\rangle$ in the third ensemble $\mathscr{E}_3 = \{h_i, |z_i\rangle\}$ to be equal to $C(\rho_{AB}^{GHZ})$, we solve the following

$$c(z_i) = \frac{\left(VYV^T\right)_{ii}}{h_i} = \lambda_1 - \lambda_2. \tag{3.100}$$

Therefore,

$$\lambda_1 V_{11}^2 - \lambda_2 V_{12}^2 = h_1 (\lambda_1 - \lambda_2), \ \lambda_1 V_{21}^2 - \lambda_2 V_{22}^2 = h_2 (\lambda_1 - \lambda_2). \tag{3.101}$$

By the orthonormality of the rows of V, we have

$$V_{11}^2 + V_{12}^2 = 1, \ \ V_{21}^2 + V_{22}^2 = 1, \quad V_{11}V_{21} = -V_{22}V_{12}. \tag{3.102}$$

Solving Eqs. (3.101) and (3.102) regarding the positivity of V, i.e., $\det V > 0$, we get

$$V = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{c_3(2h_1 - 1) + 1} & -\sqrt{c_3(1 - 2h_1) + 1} \\ \sqrt{c_3(2h_2 - 1) + 1} & \sqrt{c_3(1 - 2h_2) + 1} \end{pmatrix}. \tag{3.103}$$

Thus, the states $|z_i\rangle$ in $\mathscr{E}_3$ are obtained from the states $|y_i\rangle$ in $\mathscr{E}_2$ given by the Eqs. (3.94) and (3.95). Since the third ensemble is the optimal ensemble, we get

$$\left|\psi_j^{opt}\right\rangle = \mu_{1j}|00\rangle + \mu_{2j}|\beta_1\beta_2\rangle \quad for\ j = 1, 2 \tag{3.104}$$

with probability $p_j = h_j$ in the ensemble $\mathscr{E}^{opt} = \left\{p_j, \left|\psi_j^{opt}\right\rangle\right\}$. Here, in terms of the entries V_{ij} of V, the complex coefficients μ_{1j} and μ_{2j} are calculated as

$$\mu_{1j} = \frac{(1 + s_3 - c_3)\left(V_{j1} - iV_{j2}\right)}{N\sqrt{2p_j(1 - c_3)}}, \tag{3.105}$$

$$\mu_{2j} = \frac{z}{N\sqrt{2p_j(1 - c_3)}}\left\{V_{j1}\left[c_3(1 - c_3) + s_3^2\right] + iV_{j2}s_3[2c_3 - 1]\right\}. \tag{3.106}$$

CHAPTER 4

TRANSFORMATIONS OF MIXED STATES

As introduced in Sec. 1.8 for pure states, SLOCC transformations for mixed states can also be defined as follows: ρ_{AB} is *stochastically reducible* to ρ'_{AB} (shown by $\rho \underset{SLOCC}{\longrightarrow} \rho'$) if there are operators A and B such that

$$\rho'_{AB} = (A \otimes B)\rho\left(A^{\dagger} \otimes B^{\dagger}\right) \tag{4.1}$$

and ρ_{AB} is *stochastically equivalent* to ρ'_{AB} or *SLOCC equivalent* to ρ'_{AB} (shown by $\rho \underset{SLOCC}{\sim} \rho'$) if $\rho \underset{SLOCC}{\longrightarrow} \rho'$ and $\rho' \underset{SLOCC}{\longrightarrow} \rho$. It can be shown that ρ_{AB} is SLOCC equivalent to ρ'_{AB} iff Eq. (4.1) holds for some invertible A and B.

Let ρ_{AB} be a matrix-rank 2 state of two qubits and $\rho \underset{SLOCC}{\longrightarrow} \rho'$, then matrix rank of ρ'_{AB} is less than 2. If matrix rank of ρ'_{AB} is 1 (i.e., if ρ'_{AB} is a pure state) then one of A and B is not invertible and therefore ρ'_{AB} must unentangled. This can be shown as follows: Suppose that A is not invertible. As A is a "2×2 matrix", this implies that $A = c\,|\alpha\rangle\langle\alpha|$ for some $|\alpha\rangle \in \mathcal{H}_A$ and constant $c \in \mathbb{C}$ and therefore

$$\rho'_{AB} = (|\alpha\rangle\langle\alpha|)_A \otimes \sigma_B \tag{4.2}$$

for some 2×2 density matrix σ. It is apparent that ρ' is unentangled and uncorrelated.

Therefore we can state the following: if $\rho \underset{SLOCC}{\longrightarrow} \rho'$ with Eq. (4.1), and if ρ'_{AB} has matrix rank 2, then

$$(\rho'_{AB} \text{ has matrix rank 2}) \Leftrightarrow (A \text{ and } B \text{ are invertible})\,. \tag{4.3}$$

From now on, consider all transformations $\rho \underset{SLOCC}{\longrightarrow} \rho'$ where both ρ_{AB} and ρ'_{AB} have rank 2. In that case, $\rho' \underset{SLOCC}{\longrightarrow} \rho$ as well, because only for invertible A and B one can satisfy Eq. (4.1).

4.1 Support of ρ_{AB} as a subspace

Let ρ_{AB} be a rank 2 mixed state of a two qubit system AB. ρ_{AB} has a spectral decomposition as

$$\rho_{AB} = \sum_{i=1}^{2} p_i\,|\psi_i\rangle\langle\psi_i| \tag{4.4}$$

where $\{|\psi_i\rangle\}$ is the orthonormal set of eigenvectors of ρ_{AB} corresponding to the eigenvalues $\{p_i\}$ of ρ_{AB}. Then, there is a 2-dimensional subspace of $\mathcal{H}_{\mathcal{AB}} = \mathcal{H}_{\mathcal{A}}\otimes\mathcal{H}_{\mathcal{B}}$ called as the *support* of ρ_{AB} or $\text{supp}(\rho_{AB})$, which is defined as the linear span of its eigenvectors

$$\text{supp}(\rho_{AB}) = \text{span}\{|\psi_1\rangle, |\psi_2\rangle\}\,. \tag{4.5}$$

Any two-dimensional subspace of $\mathcal{H}_{\mathcal{AB}}$ always contains a product state, of which detailed proof is given by Sampera, Tarrach, and Vidal [58].

There are two nontrivial cases we can think of:

1. *Class* $\mathbb{P}_1$. All the product states $\text{supp}(\rho_{AB})$ contains are parallel. Hence if

$$|a\rangle = |\alpha_1\rangle_A \otimes |\alpha_2\rangle_B \tag{4.6}$$

   is *the* product state in $\text{supp}(\rho_{AB})$, then $\text{supp}(\rho_{AB})$ does not contain any other product state that is linearly independent of $|a\rangle$. In such a case, we can find an entangled state $|b\rangle$ such that $\{|a\rangle, |b\rangle\}$ is a basis of $\text{supp}(\rho_{AB})$.

2. *Class* $\mathbb{P}_2$. In this case, $\text{supp}(\rho_{AB})$ contains two linearly independent product states. Call these

$$|a\rangle = |\alpha_1\rangle_A \otimes |\alpha_2\rangle_B \text{ and } |b\rangle = |\beta_1\rangle_A \otimes |\beta_2\rangle_B . \tag{4.7}$$

   Therefore, any vector in $\text{supp}(\rho_{AB})$ can be written as a superposition of these.

In short, in both cases, one can find a basis $\{|a\rangle, |\phi\rangle\}$ of $\text{supp}(\rho_{AB})$ such that $|a\rangle$ is a product state.

Now, we consider alternative representations of ρ_{AB} in the form

$$\rho_{AB} = \sum_{i=1}^{2} |u_i\rangle\langle u_i\rangle = \sum_{i=1}^{2} |u'_i\rangle\langle u'_i\rangle$$

where Eq. (4.4) is a special example. In all of these examples, $\{|u_1\rangle, |u_2\rangle\}$ (similarly, $\{|u'_1\rangle, |u'_2\rangle\}$) spans the support of ρ_{AB}. In fact they form alternative bases for the support. By Schrödinger-HJW theorem, these alternative representations are related by $|u'_i\rangle = \sum_j V_{ij} |u'_j\rangle$. Recall that the dimension of the unitary V depends on the number of elements in the corresponding sets and therefore, it is taken 2×2 in this case. This type of ensembles are called *minimal ensembles* which contains only n states to represent rank n mixed states [36].

A special case is the subnormalized states $|\psi_i^{sub}\rangle = \sqrt{p_i}|\psi_i\rangle$ where $|\psi_i\rangle$ are the eigenvectors and p_i are the eigenvalues of ρ_{AB}, then

$$\sum_{i=1}^{2} |\psi_i^{sub}\rangle\langle\psi_i^{sub}| = \sum_{i=1}^{2} p_i |\psi_i\rangle\langle\psi_i| = \rho_{AB}. \tag{4.8}$$

Now, suppose that an unnormalized product state $|P\rangle$ in $\text{supp}(\rho_{AB})$ is parallel to the product state $|a\rangle$ defined by Eq. (4.6). $|P\rangle$ can be written as a linear combination of $\{|\psi_1^{sub}\rangle, |\psi_2^{sub}\rangle\}$ such that

$$|P\rangle = \kappa|a\rangle = d_1 |\psi_1^{sub}\rangle + d_2 |\psi_2^{sub}\rangle \tag{4.9}$$

for some complex numbers κ, d_1 and d_2. Here, we require that $\{d_1, d_2\}$ satisfies $|d_1|^2 + |d_2|^2 = 1$. Note that

$$\||P\rangle\|^2 = p_1 |d_1|^2 + p_2 |d_2|^2 \leq 1 \tag{4.10}$$

since $\left\| |\psi_1^{sub}\rangle \right\| = \sqrt{p_i}$. Now, define a unitary

$$V = \begin{bmatrix} d_1 & d_2 \\ -d_2^* & d_1^* \end{bmatrix}. \tag{4.11}$$

It can be seen that this is a unitary matrix because its columns (also rows) form an orthonormal set. For another set of states $\{|u_i\rangle\}$ which realizes ρ_{AB}, it is true that $|u_i\rangle = \sum_{j=1}^{n} V_{ij} \left|\psi_j^{sub}\right\rangle$ then $|u_1\rangle = |P\rangle = \kappa |a\rangle$. Therefore, one can always find a representation $\{|u_i\rangle\}$ of ρ_{AB} where one of the states $|u_1\rangle$ is parallel to a given product state $|a\rangle$. Also, $|u_2\rangle$ will be some other state in $\operatorname{supp}(\rho_{AB})$ which is

$$|u_2\rangle = -d_2^* \left|\psi_1^{sub}\right\rangle + d_1^* \left|\psi_2^{sub}\right\rangle \tag{4.12}$$

so that

$$\sum_{i=1}^{2} |u_i\rangle \langle u_i| = \sum_{i=1}^{2} \left|\psi_i^{sub}\right\rangle \left\langle \psi_i^{sub}\right| = \rho_{AB}. \tag{4.13}$$

4.2 States with class $\mathbb{P}_1$ supports

Consider all representations of ρ_{AB}

$$\rho_{AB} = |u_1\rangle \langle u_1| + |u_2\rangle \langle u_2| \tag{4.14}$$

where $|u_1\rangle = \kappa |a\rangle$ for some product state $|a\rangle$ and $|u_2\rangle$ is necessarily entangled if $\operatorname{supp}(\rho_{AB})$ is of class $\mathbb{P}_1$. Moreover, $|u_2\rangle + z |u_1\rangle$ are always entangled for all $z \in \mathbb{C}$. Let

$$\rho_{AB} = \left|u_1'\right\rangle \left\langle u_1'\right| + \left|u_2'\right\rangle \left\langle u_2'\right| \tag{4.15}$$

be another representation of ρ_{AB} such that $\left|u_1'\right\rangle$ is a product state. In this case, since $\operatorname{supp}(\rho_{AB})$ contains only one non-parallel product state, we necessarily have $\left|u_1'\right\rangle = \kappa' |a\rangle$ for some number κ'. Because of the Schrödinger-HJW theorem we also know that then there is a unitary V such that $\left|u_1'\right\rangle = V_{11} |u_1\rangle + V_{12} |u_2\rangle$. But, if V_{12} were nonzero, then $\left|u_1'\right\rangle$ would have been entangled. However, it is chosen as a product state, so $V_{12} = 0$ necessarily and therefore V is diagonal. Then

$$\left|u_i'\right\rangle = e^{i\theta_i} |u_i\rangle \quad (i = 1, 2) \tag{4.16}$$

The states are identical up to an overall phase factor.

In conclusion, if ρ_{AB} is such that $\operatorname{supp}(\rho_{AB})$ contains at most one linearly independent product state, then, the decomposition of ρ_{AB} given by Eq. (4.14) such that $|u_1\rangle$ is a product state is unique up to overall phases of $|u_1\rangle$ and $|u_2\rangle$.

Let ρ_{AB} be of class $\mathbb{P}_1$. One can then find a basis $\{|\alpha_0\rangle, |\alpha_1\rangle\}$ of $\mathcal{H}_A = \mathbb{C}^2$ and a basis $\{|\beta_0\rangle, |\beta_1\rangle\}$ of $\mathcal{H}_B = \mathbb{C}^2$ such that $\rho_{AB} = |u_1\rangle \langle u_1| + |u_2\rangle \langle u_2|$ where

$$\begin{aligned} |u_1\rangle_{AB} &= |\alpha_0\rangle_A \otimes |\beta_0\rangle_B, \\ |u_2\rangle_{AB} &= |\alpha_0\rangle_A \otimes |\beta_1\rangle_B + |\alpha_1\rangle_A \otimes |\beta_0\rangle_B. \end{aligned} \tag{4.17}$$

Unfortunately, this representation is not unique. Let $\rho_{AB} = \left|u_1'\right\rangle \left\langle u_1'\right| + \left|u_2'\right\rangle \left\langle u_2'\right|$ where

$$\begin{aligned} \left|u_1'\right\rangle &= e^{i\theta_1} |u_1\rangle = \left|\alpha_0'\right\rangle \otimes \left|\beta_0'\right\rangle, \\ \left|u_2'\right\rangle &= e^{i\theta_2} |u_2\rangle = \left|\alpha_0'\right\rangle \otimes \left|\beta_1'\right\rangle + \left|\alpha_1'\right\rangle \otimes \left|\beta_0'\right\rangle \end{aligned} \tag{4.18}$$

then

$$\begin{aligned} \left|\alpha_0'\right\rangle &= z |\alpha_0\rangle, \\ \left|\beta_0'\right\rangle &= \frac{e^{i\theta_1}}{z} |\beta_0\rangle, \\ \left|\beta_1'\right\rangle &= \frac{e^{i\theta_2} |\beta_1\rangle - \lambda |\beta_0\rangle}{z}, \\ \left|\alpha_1'\right\rangle &= z e^{-i\theta_1} \left(e^{i\theta_2} |\alpha_1\rangle + \lambda |\alpha_0\rangle\right) \end{aligned} \tag{4.19}$$

where $z \neq 0$, $\lambda \in \mathbb{C}$, $\theta_1, \theta_2 \in \mathbb{R}$ are arbitrary.

Let ρ_{AB} and ρ'_{AB} be of class $\mathbb{P}_1$. Can we stochastically reduce ρ_{AB} to ρ'_{AB}, i.e., $\rho \underset{SLOCC}{\overset{?}{\longrightarrow}} \rho'$? We will show below that the answer is affirmative. Let $\rho_{AB} = \sum_{i=1}^{2} |u_i\rangle\langle u_i|$, $\rho'_{AB} = \sum_{i=1}^{2} |u'_i\rangle\langle u'_i|$ and let

$$\begin{aligned} |u_1\rangle &= |\alpha_0\rangle \otimes |\beta_0\rangle, \\ |u_2\rangle &= |\alpha_0\rangle \otimes |\beta_1\rangle + |\alpha_1\rangle \otimes |\beta_0\rangle, \\ |u'_1\rangle &= |\alpha'_0\rangle \otimes |\beta'_0\rangle, \\ |u'_2\rangle &= |\alpha'_0\rangle \otimes |\beta'_1\rangle + |\alpha'_1\rangle \otimes |\beta'_0\rangle. \end{aligned} \tag{4.20}$$

Can one find local operators A and B such that $(A \otimes B)|u_i\rangle = |u'_i\rangle$ $(i, j = 2)$? The problem can be solved by finding A and B such that

$$A|\alpha_i\rangle = |\alpha'_i\rangle, \qquad B|\beta_i\rangle = |\beta'_i\rangle. \tag{4.21}$$

The local operators A and B that satisfy these are not unique. In general, one can find A and B such that

$$\begin{aligned} A|\alpha_0\rangle &= z|\alpha'_0\rangle, \\ A|\alpha_1\rangle &= ze^{-i\theta_1}\left(e^{i\theta_2}|\alpha'_1\rangle + \lambda|\alpha'_0\rangle\right), \\ B|\beta_0\rangle &= \frac{e^{i\theta_1}}{z}|\beta'_0\rangle, \\ B|\beta_1\rangle &= \frac{e^{i\theta_2}|\beta'_1\rangle - \lambda|\beta'_0\rangle}{z} \end{aligned} \tag{4.22}$$

for any given $z \neq 0, \lambda \in \mathbb{C}, \theta_1, \theta_2 \in \mathbb{R}$. For all of such A and B the relation $\rho'_{AB} = (A \otimes B)\rho\left(A^\dagger \otimes B^\dagger\right)$ is satisfied. This proves the claim, i.e., any two states ρ_{AB} and ρ'_{AB} having supports of class $\mathbb{P}_2$ are SLOCC equivalent. Therefore, all density matrices with supports of class $\mathbb{P}_2$ form a SLOCC class.

4.3 States with class $\mathbb{P}_2$ supports

Let $|a\rangle$ and $|b\rangle$ be two linearly independent product states given by Eq. (4.7). Then, either $\{|\alpha_1\rangle_A, |\beta_1\rangle_A\}$ is linearly independent or $\{|\alpha_2\rangle_B, |\beta_2\rangle_B\}$ is linearly independent or both. There are three cases that one can distinguish.

1. *Class $\mathbb{P}_{2B}$ (only B is mixed):* While $\{|\alpha_1\rangle_A, |\beta_1\rangle_A\}$ is linearly dependent, $\{|\alpha_2\rangle_B, |\beta_2\rangle_B\}$ is linearly independent. For this case, $|\alpha_2\rangle$ is parallel to $|\alpha_1\rangle$, and all states in $\mathrm{supp}(\rho_{AB})$ is of the form $|\alpha_1\rangle_A \otimes |\psi\rangle_B$ where $|\psi\rangle_B$ is arbitrary. Therefore, ρ_{AB} is unentangled and uncorrelated, with A being in a pure state $|\alpha_1\rangle_A$ and B is in a mixed state (say σ)

$$\rho_{AB} = (|\alpha_1\rangle\langle\alpha_1|)_A \otimes \sigma_B. \tag{4.23}$$

2. *Class $\mathbb{P}_{2A}$ (only A is mixed):* While $\{|\alpha_2\rangle_B, |\beta_2\rangle_B\}$ is linearly dependent, $\{|\alpha_1\rangle_A, |\beta_1\rangle_A\}$ is linearly independent. For this case, $|\beta_2\rangle$ is parallel to $|\alpha_2\rangle$ and all states in $\mathrm{supp}(\rho_{AB})$ is of the form $|\psi\rangle_A \otimes |\alpha_2\rangle_B$ where $|\psi\rangle_A$ is arbitrary. ρ_{AB} is unentangled and uncorrelated, with B being in a pure state $|\alpha_2\rangle_B$ and A is in a mixed state (say σ)

$$\rho_{AB} = \sigma_A \otimes (|\alpha_2\rangle\langle\alpha_2|)_B. \tag{4.24}$$

3. *Class $\mathbb{P}_{2AB}$ (both A and B are mixed):* Both $\{|\alpha_1\rangle_A, |\beta_1\rangle_A\}$ and $\{|\alpha_2\rangle_B, |\beta_2\rangle_B\}$ are linearly independent. This implies that the generic state
$$|\psi\rangle \quad = c_1 |a\rangle + c_2 |b\rangle = c_1 |\alpha_1\rangle_A \otimes |\beta_1\rangle_B + c_2 |\alpha_2\rangle_A \otimes |\beta_2\rangle_B \tag{4.25}$$
is always entangled for $c_1 \neq 0$, $c_2 \neq 0$.

It can be shown that all states having supports of class $\mathbb{P}_{2A}$ and those that have supports of class $\mathbb{P}_{2B}$ do form separate SLOCC classes. The case of $\mathbb{P}_{2AB}$ is highly non-trivial and is studied in detail below.

If $|u\rangle \in \operatorname{supp}(\rho_{AB})$ and $|u\rangle$ is a product state then either $|u\rangle = N|a\rangle$ or $|u\rangle = N|b\rangle$ for some complex number N. So if ρ_{AB} is of type given by Eq. (4.14) and $|u_1\rangle$ is a product state, then either $|u_1\rangle$ is parallel to $|a\rangle$ or to $|b\rangle$. Consider two possible representations of ρ_{AB},
$$\rho_{AB} = |u_1\rangle\langle u_1| + |u_2\rangle\langle u_2| = |u_1'\rangle\langle u_1'| + |u_2\rangle\langle u_2'| \tag{4.26}$$
where $|u_1\rangle$ and $|u_1'\rangle$ are product states. If $|u_1\rangle$ is parallel to $|u_1'\rangle$ then we have
$$|u_i'\rangle = e^{i\theta_i} |u_i\rangle, \tag{4.27}$$
i.e., the states in the two ensembles are identical up to an overall phase factor.

Now, consider the case where $|u_1\rangle$ is parallel to $|a\rangle$ and $|u_1'\rangle$ is parallel to $|b\rangle$. Let
$$|u_1\rangle = x|a\rangle \tag{4.28}$$
(where x is real and $x > 0$) and
$$|u_2\rangle = y|a\rangle + z|b\rangle. \tag{4.29}$$
We can choose y to be real and $y \geq 0$. Obviously $z \neq 0$. Thus,
$$\begin{aligned}\rho_{AB} &= \sum_{i=1}^{2} |u_i\rangle\langle u_i| \\ &= \left(x^2 + y^2\right)|a\rangle\langle a| + yz|b\rangle\langle a| \\ &+yz^*|a\rangle\langle b| + |z|^2|b\rangle\langle b|.\end{aligned} \tag{4.30}$$
Similarly, let
$$|u_1'\rangle = x'|b\rangle \tag{4.31}$$
and
$$|u_2'\rangle = y'|b\rangle + z'|a\rangle \tag{4.32}$$
where x' and y' are real, $x' > 0$ and $y' \geq 0$, and again, $z' \neq 0$. Thus,
$$\begin{aligned}\rho_{AB} &= \sum_{i=1}^{2} |u_i'\rangle\langle u_i'| \\ &= |z'|^2 |a\rangle\langle a| + y'z'|a\rangle\langle b| \\ &+y'z'^*|b\rangle\langle a| + \left(x'^2 + y'^2\right)|b\rangle\langle b|\end{aligned} \tag{4.33}$$
then
$$\begin{aligned}|z'|^2 &= x^2 + y^2, \\ y'z' &= yz^*, \\ x'^2 + y'^2 &= |z|^2.\end{aligned} \tag{4.34}$$

If the expansion of ρ_{AB} is known, one can select the overall phase of $|b\rangle$ (relative to that of $|a\rangle$) such that z is real and positive.

Let

$$\rho_{AB} = R_{11}\,|a\rangle\langle a| + R_{12}\,(|a\rangle\langle b| + |b\rangle\langle a|) + R_{22}\,|a\rangle\langle b| \tag{4.35}$$

where the overall phases of $|b\rangle$ and $|a\rangle$ have been redefined such that R_{12} is real and positive. Then,

$$\begin{aligned} x^2 + y^2 = z'^2 &= R_{11}, \\ yz = y'z' &= R_{12}, \\ z^2 = x'^2 + y'^2 &= R_{22} \end{aligned} \tag{4.36}$$

$$\begin{aligned} &\Rightarrow z \equiv \sqrt{R_{12}},\, z' \equiv \sqrt{R_{11}}, \\ &y \equiv \frac{R_{12}}{\sqrt{R_{22}}},\; y' \equiv \frac{R_{12}}{\sqrt{R_{11}}}, \\ &x \equiv \sqrt{R_{11} - \frac{R_{12}^2}{R_{22}}} = \sqrt{\frac{\det R}{R_{22}}},\; x' \equiv \sqrt{\frac{\det R}{R_{11}}}. \end{aligned} \tag{4.37}$$

Note that even though the phases of $|a\rangle$ and $|b\rangle$ are adjusted such that R_{12} is real and positive, the inner product $\langle a\,|b\,\rangle$ might still have a phase.

4.4 SLOCC classes

Let $\rho \underset{SLOCC}{\sim} \rho'$, then

$$\begin{pmatrix} \text{supp}\,(\rho_{AB}) \text{ contains} \\ \text{2 linearly independent} \\ \text{product states (i.e., } \rho_{AB} \text{ is} \\ \text{of class } \mathbb{P}_2) \end{pmatrix} \Leftrightarrow \begin{pmatrix} \text{supp}\,(\rho'_{AB}) \text{ contains} \\ \text{2 linearly independent} \\ \text{product states (i.e., } \rho'_{AB} \text{ is} \\ \text{of class } \mathbb{P}_2) \end{pmatrix}. \tag{4.38}$$

Let us show this implication. Let $\rho_{AB} = \sum_{i=1}^{2} |u_i\rangle\langle u_i|$ and $\rho'_{AB} = \sum_{i=1}^{2} \left|u'_i\right\rangle\left\langle u'_i\right|$ be representatives where $|u_1\rangle$ and $\left|u'_1\right\rangle$ are product states and let $\rho'_{AB} = (A \otimes B)\,\rho\left(A^\dagger \otimes B^\dagger\right)$. Let us first show the forward implication (($\Rightarrow$:) Suppose ρ_{AB} is of class $\mathbb{P}_2$, so

$$\begin{aligned} |u_1\rangle &= x\,|a\rangle\,, \\ |u_2\rangle &= y\,|a\rangle + z\,|b\rangle \end{aligned} \tag{4.39}$$

where $|a\rangle$ and $|b\rangle$ are product states. Define

$$\begin{aligned} |\tilde{a}\rangle &= A \otimes B\,|a\rangle\,, \\ \left|\tilde{b}\right\rangle &= A \otimes B\,|b\rangle\,, \end{aligned} \tag{4.40}$$

that is, $|\tilde{a}\rangle$ and $\left|\tilde{b}\right\rangle$ are product states. Then,

$$\begin{aligned} |\tilde{u}_1\rangle &= x\,|\tilde{a}\rangle\,, \\ |\tilde{u}_2\rangle &= y\,|\tilde{a}\rangle + z\left|\tilde{b}\right\rangle \end{aligned} \tag{4.41}$$

$$\Rightarrow \rho'_{AB} = \sum_{i=1}^{2} \left|\widetilde{u_i}'\right\rangle\left\langle\widetilde{u_i}'\right| \tag{4.42}$$

so ρ_{AB} is also in class $\mathbb{P}_2$. The reverse implication ($\Leftarrow$:) is obvious as this is equivalent to $\rho' \underset{SLOCC}{\longrightarrow} \rho$.

If $\rho \underset{SLOCC}{\sim} \rho'$, *then*

$$(\rho_{AB} \textit{ is of class } \mathbb{P}_1) \Leftrightarrow (\rho'_{AB} \textit{ is of class } \mathbb{P}_1)\,. \tag{4.43}$$

This has been shown somewhere above. In general, if $\rho \underset{SLOCC}{\sim} \rho'$ *then*

1. $\rho_{AB} \in \mathbb{P}_1 \Leftrightarrow \rho'_{AB} \in \mathbb{P}_1$,
2. $\rho_{AB} \in \mathbb{P}_2 \Leftrightarrow \rho'_{AB} \in \mathbb{P}_2$,
3. $\rho_{AB} \in \mathbb{P}_{2A} \Leftrightarrow \rho'_{AB} \in \mathbb{P}_{2A}$,
4. $\rho_{AB} \in \mathbb{P}_{2B} \Leftrightarrow \rho'_{AB} \in \mathbb{P}_{2B}$,
5. $\rho_{AB} \in \mathbb{P}_{2AB} \Leftrightarrow \rho'_{AB} \in \mathbb{P}_{2AB}$.

Let ρ_{AB} be of class $\mathbb{P}_1$, $\rho_{AB} = \sum_{i=1}^{2} |u_i\rangle\langle u_i|$ and

$$|u_1\rangle = c\,|a\rangle_{AB} = c\,|\alpha_1\rangle_A \otimes |\alpha_2\rangle_B\,. \tag{4.44}$$

Now, redefine $|\alpha_1\rangle$ or $|\alpha_2\rangle$ such that $c = 1$, then

$$|u_1\rangle = |a\rangle_{AB} = |\alpha_1\rangle_A \otimes |\alpha_2\rangle_B\,. \tag{4.45}$$

Let $\{|\alpha_1\rangle_A, |\beta_1\rangle_A\}$ be a basis of $\mathcal{H}_{\mathcal{A}} = \mathbb{C}^2$ and $\{|\alpha_2\rangle_B, |\beta_2\rangle_B\}$ be a basis of $\mathcal{H}_{\mathcal{B}} = \mathbb{C}^2$. Let

$$\begin{aligned} |u_2\rangle &= d\,|\alpha_1 \otimes \alpha_2\rangle + e\,|\beta_1 \otimes \alpha_2\rangle \\ &\quad + f\,|\alpha_1 \otimes \beta_2\rangle + g\,|\beta_1 \otimes \beta_2\rangle\,. \end{aligned} \tag{4.46}$$

Here

$$\det\begin{bmatrix} d+z & e \\ f & g \end{bmatrix} \neq 0 \text{ for all } z. \tag{4.47}$$

This implies that $g = 0$ (otherwise ρ_{AB} is of class $\mathbb{P}_2$). Then

$$|u_2\rangle = d\,|\alpha_1 \otimes \alpha_2\rangle + e\,|\beta_1 \otimes \alpha_2\rangle + f\,|\alpha_1 \otimes \beta_2\rangle\,. \tag{4.48}$$

Redefine $|\beta_1\rangle$ and $|\beta_2\rangle$ as follows:

$$\begin{aligned} \left|\tilde{\beta}_1\right\rangle &= e\,|\beta_1\rangle + \lambda\,|\alpha_1\rangle\,, \\ \left|\tilde{\beta}_2\right\rangle &= f\,|\beta_2\rangle + \mu\,|\alpha_2\rangle \end{aligned} \tag{4.49}$$

$$\Rightarrow |u_2\rangle = (d - \lambda - \mu)\,|\alpha_1 \otimes \alpha_2\rangle + \left|\tilde{\beta}_1 \otimes \alpha_2\right\rangle + \left|\alpha_1 \otimes \tilde{\beta}_2\right\rangle \tag{4.50}$$

for given λ, select $\mu = d - \lambda$ which leads to the following corollary:

Let ρ_{AB} be of class $\mathbb{P}_{2AB}$. There is a basis $\{|\alpha_0\rangle, |\alpha_1\rangle\}$ of $\mathcal{H}_{\mathcal{A}} = \mathbb{C}^2$ and a basis $\{|\beta_0\rangle, |\beta_1\rangle\}$ of $\mathcal{H}_{\mathcal{B}} = \mathbb{C}^2$ such that $\rho_{AB} = |u_1\rangle\langle u_1| + |u_2\rangle\langle u_2|$ where

$$\begin{aligned} |u_1\rangle &= c_1\,|\alpha_0\rangle \otimes |\beta_0\rangle\,, \\ |u_2\rangle &= c_2\,|\alpha_0\rangle \otimes |\beta_0\rangle + c_3\,|\alpha_1\rangle \otimes |\beta_1\rangle\,. \end{aligned} \tag{4.51}$$

In general, one can absorb c_1, c_2, and c_3 into the definitions of $|\alpha_i\rangle$, $|\beta_i\rangle$. But, $|c_2/c_1|$ can not be changed by such redefinitions.

$$\begin{aligned} |u_1\rangle &= |\alpha_0\rangle \otimes |\beta_0\rangle \\ |u_2\rangle &= k\,|\alpha_0\rangle \otimes |\beta_0\rangle + |\alpha_1\rangle \otimes |\beta_1\rangle \end{aligned} \tag{4.52}$$

where k is real with $k \geq 0$.

Note that a purification of ρ_{AB} is

$$\begin{aligned} |\psi\rangle_{ABC} &= |u_1\rangle_{AB} \otimes |1\rangle_C + |u_2\rangle_{AB} \otimes |0\rangle_C \\ &= |\alpha_1 \otimes \beta_1 \otimes 0\rangle + |\alpha_1 \otimes \beta_1\rangle \otimes (k\,|0\rangle + |1\rangle) \end{aligned} \tag{4.53}$$

where

$$\frac{k}{\sqrt{k^2+1}} = c_3 \text{ or } k = \frac{c_3}{\sqrt{1-c_3^2}} = \frac{c_3}{s_3} \tag{4.54}$$

requirement is $k \neq \infty$ ($c_3 \neq 1$). Hence the parameter k is related to the cosine c_3 of 3^{rd} party C. Let $\rho_{AB}, \rho'_{AB} \in \mathbb{P}_{2AB}$. $\rho \underset{SLOCC}{\longrightarrow} \rho'$ iff $k \neq k'$. The parameter k can not change in stochastic transformations.

CHAPTER 5

CONCLUSION

In the 2^{nd} chapter, Wootters' concurrence [54], which is a good measure of entanglement, is determined for partially entangled bipartite pure states, i.e., states of the form $\alpha|00\rangle + \beta|11\rangle$. After that, the concurrence is calculated for two qubit mixed states that have matrix rank 2. For these states, the state can be expressed as the reduced density matrix of a tripartite entangled state of three qubits. Using known standard expressions for the W class and GHZ class states of three qubits, expressions for the concurrence of two qubits are obtained.

In the 3^{rd} chapter, Wootters' method for finding optimal ensembles [54] is used on rank 2 mixed states of two qubits. As expressing the eigenvectors of these density matrices is usually complicated (this is especially true for the states whose purifications are in GHZ class (see Appendix A)), a slightly different approach is followed for some of the computations.

In the 4^{th} chapter, the SLOCC classification of the mixed states of two qubits is investigated. All of the SLOCC classes of rank 2 mixed states are identified. To achieve this, first the supports of the mixed states, and their properties that remain invariant under stochastic reducibility relation is investigated. The relevant properties of these subspaces turn out to be the number of non-parallel product states in the support. There appeared to be 3 different situations for rank 2 mixed states. Either there is only one product state in the support, in which case all such mixed states form a single SLOCC class. There can be two (and only two) non-parallel product states in the support, in which case there is a real variable that remains invariant under stochastic reducibility. Thus, there are infinitely many SLOCC classes in this case; the classes depend on a real parameter. Finally, it is possible to find infinitely many product states in the support, in which case the mixed state itself is necessarily a product state. There can not be any entanglement in that case.

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APPENDIX A

OPTIMAL ENSEMBLE REPRESENTING ρ_{AB}^{GHZ} STARTING WITH SPECTRAL DECOMPOSITION

To find the eigenvalues and the eigenstates of the mixed state ρ_{AB}^{GHZ} of the composite system AB, consult the tool of Schmidt decomposition of $|\Psi\rangle_{ABC}$ as $AB - C$ which is used in the following sections.

A.1 Schmidt decomposition of $|\Psi\rangle_{ABC}$ as $AB - C$

Consider the tripartite system ABC as the composition of the $AB - C$ where AB and C are defined on the Hilbert spaces $\mathcal{H}_{AB}^{\otimes 4}$ and $\mathcal{H}_{C}^{\otimes 2}$, respectively. Therefore, it is to say that eigenvalues of the subsystems AB and C are the same and then that

$$n_{\psi} \leq \min(4, 2) = 2 \tag{A.1}$$

which means that ranks of ρ_{AB}^{GHZ} and ρ_{C}^{GHZ} are at most 2. For this reason, it is more convenient to deal with the eigenvalues and eigenvectors of 2×2 matrix ρ_{C}^{GHZ} rather than the 4×4 matrix ρ_{AB} [36,41,59].

ρ_{C}^{GHZ} is calculated by partial tracing the party AB from the total state $|\Psi\rangle_{ABC}$, namely

$$\begin{aligned} \rho_{C}^{GHZ} &= \mathrm{tr}_C \left(|\Psi\rangle\langle\Psi|\right)_{ABC} \\ &= \||a_1\rangle\|^2 |0\rangle\langle 0| + \langle a_2 | a_1 \rangle |0\rangle\langle 1| \\ &\quad + \langle a_1 | a_2 \rangle |1\rangle\langle 0| + \||a_2\rangle\|^2 |1\rangle\langle 1| \end{aligned} \tag{A.2}$$

which can also be given a matrix representation

$$\rho_{C}^{GHZ} = \begin{pmatrix} \||a_1\rangle\|^2 & \langle a_1 | a_2 \rangle^* \\ \langle a_1 | a_2 \rangle & \||a_2\rangle\|^2 \end{pmatrix} \tag{A.3}$$

in the computational basis set $\{|0\rangle, |1\rangle\}$. The set of eigenvalues μ_i are the solution of the characteristic equation

$$\begin{aligned} c(\mu) &= \det\left(\rho_{C}^{GHZ} - \mu I\right) \\ &= \mu^2 - \mu + \||a_1\rangle\|^2 \||a_2\rangle\|^2 - |\langle a_1 | a_2 \rangle|^2 = 0 \end{aligned} \tag{A.4}$$

so that

$$\mu_{1,2} = \frac{1 \pm \sqrt{\triangle}}{2}. \tag{A.5}$$

where $\triangle$ is the discriminant defined by

$$\triangle = 1 - 4\frac{|z|^2 s_3^2}{N^4}\left\{1 - c_1^2 c_2^2\right\}. \tag{A.6}$$

Schmidt decomposition given by Eq. (1.28) for $|\Psi\rangle_{ABC}$ of the system ABC into the subsystems $AB-C$ gives

$$|\Psi\rangle_{ABC} = \sum_{i=1}^{2} \sqrt{\mu_i}\, |i_{AB}\rangle \otimes |i_C\rangle \tag{A.7}$$

where $|i_{AB}\rangle$ and $|i_C\rangle$ are orthonormal set of the eigenstates of ρ_{AB}^{GHZ} and ρ_{C}^{GHZ}, respectively, corresponding to the eigenvalues μ_i's in the decreasing order. One can represent the states $|0\rangle$ and $|1\rangle$ in the orthonormal basis set $|1_C\rangle$ and $|2_C\rangle$ such that

$$\begin{aligned} |0\rangle &= \underbrace{\langle 1_C\, |0\rangle}_{x_1} |1_C\rangle + \underbrace{\langle 2_C\, |0\rangle}_{x_2} |2_C\rangle \\ &= x_1\, |1_C\rangle + x_2\, |2_C\rangle \end{aligned} \tag{A.8}$$

and

$$\begin{aligned} |1\rangle &= \underbrace{\langle 1_C\, |1\rangle}_{y_1} |1_C\rangle + \underbrace{\langle 2_C\, |1\rangle}_{y_2} |2_C\rangle \\ &= y_1\, |1_C\rangle + y_2\, |2_C\rangle \end{aligned} \tag{A.9}$$

noting that

$$|i_C\rangle = \begin{pmatrix} m_i \\ n_i \end{pmatrix} = \begin{pmatrix} \langle 0\, |i_C\rangle \\ \langle 1\, |i_C\rangle \end{pmatrix} = \begin{pmatrix} x_i^* \\ y_i^* \end{pmatrix}. \tag{A.10}$$

Putting these values into Eq. 2.41 and then expanding also Eq. (A.7), we get

$$\begin{aligned} |\Psi\rangle_{ABC} &= |a_1\rangle \otimes |0\rangle + |a_2\rangle \otimes |1\rangle \\ &= (x_1\, |a_1\rangle + y_1\, |a_2\rangle) \otimes |1_C\rangle \\ &+ (x_2\, |a_1\rangle + y_2\, |a_2\rangle) \otimes |2_C\rangle & \text{(A.11)} \\ &= \sqrt{\mu_1}\, |1_{AB}\rangle \otimes |1_C\rangle + \sqrt{\mu_2}\, |2_{AB}\rangle \otimes |2_C\rangle & \text{(A.12)} \end{aligned}$$

equating Eqn.s (A.11) and (A.12) gives the eigenstates $|i_{AB}\rangle$ of ρ_{AB}^{GHZ} in terms of the coefficients of the eigenstates $|i_C\rangle$ of ρ_C^{GHZ} and the vectors $|a_1\rangle$ and $|a_2\rangle$ as the following

$$|i_{AB}\rangle = \frac{1}{\sqrt{\mu_i}} \{x_i\, |a_1\rangle + y_i\, |a_2\rangle\} \tag{A.13}$$

or

$$|i_{AB}\rangle = \frac{1}{\sqrt{\mu_i}} \{m_i^*\, |a_1\rangle + n_i^*\, |a_2\rangle\}. \tag{A.14}$$

Eigenstates $|i_C\rangle$ of ρ_C^{GHZ} are determined by the eigenvector-eigenvalue relation

$$\rho_C^{GHZ}\, |i_C\rangle = \mu_i\, |i_C\rangle \tag{A.15}$$

as

$$|i_C\rangle = \frac{1}{N_i} \begin{pmatrix} m_i \\ n \end{pmatrix} = \frac{1}{\sqrt{\pm\sqrt{\triangle}\left(\mu_i - \||a_2\rangle\|^2\right)}} \begin{pmatrix} \mu_i - \||a_2\rangle\|^2 \\ \langle a_1\, |a_2\rangle \end{pmatrix} \tag{A.16}$$

where N_i is found as the following:

$$\begin{aligned} N_i^2 &= |m_i|^2 + |n|^2 \\ &= \mu_i^2 + \||a_2\rangle\|^4 - 2\mu_i\, \||a_2\rangle\|^2 + |\langle a_1\, |a_2\rangle|^2 \end{aligned} \tag{A.17}$$

adding $c(\mu_i) = \mu_i^2 - \mu_i + \||a_1\rangle\|^2 \||a_2\rangle\|^2 - |\langle a_1 | a_2 \rangle|^2 = 0$ which is characteristic equation given by Eq. (A.4) to the right side gives

$$\begin{aligned} N_i^2 &= \left(\mu_i - \||a_2\rangle\|^2\right) \underbrace{(2\mu_i - 1)}_{\pm\sqrt{\triangle}} \\ &= \pm\sqrt{\triangle}\left(\mu_i - \||a_2\rangle\|^2\right). \end{aligned} \tag{A.18}$$

Finally, the eigenvectors $|i_{AB}\rangle$ of ρ_{AB}^{GHZ} become

$$|i_{AB}\rangle = \frac{\left(\mu_i - \||a_2\rangle\|^2\right)|a_1\rangle + \langle a_1 | a_2 \rangle^* |a_2\rangle}{\sqrt{\pm\mu_i\sqrt{\triangle}\left(\mu_i - \||a_2\rangle\|^2\right)}} \tag{A.19}$$

Subnormalization of $|i_{AB}\rangle$ is defined by $\langle i_{AB} | i_{AB} \rangle = \mu_i$ which results in the subnormalized eigenstates

$$|i_{AB}\rangle_{sub} = \frac{\left(\mu_i - \||a_2\rangle\|^2\right)|a_1\rangle + \langle a_1 | a_2 \rangle^* |a_2\rangle}{\sqrt{\pm\sqrt{\triangle}\left(\mu_i - \||a_2\rangle\|^2\right)}} \tag{A.20}$$

or simply

$$|i_{AB}\rangle_{sub} = d_i\left(m_i |a_1\rangle + n^* |a_2\rangle\right) \tag{A.21}$$

where

$$d_i = N_i^{-1}. \tag{A.22}$$

A.2 The first decomposition of ρ_{AB}^{GHZ}

Start with the spectral decomposition of ρ_{AB}^{GHZ}

$$\rho_{AB}^{GHZ} = \sum_{i=1}^{2} \mu_i |i_{AB}\rangle\langle i_{AB}| \tag{A.23}$$

or in terms of the subnormalized eigenstates $|i_{AB}\rangle_{sub} \equiv \sqrt{\mu_i}\,|i_{AB}\rangle$

$$\rho_{AB}^{GHZ} = \sum_{i=1}^{2} |i_{AB}\rangle_{sub}\langle i_{AB}|_{sub}. \tag{A.24}$$

There is a unitary matrix U that transforms the states $|i_{AB}\rangle_{sub}$ to another set of states $|w_i\rangle_{sub}$ with the formula

$$|w_i\rangle_{sub} = \sum_{i=1}^{2} U_{ij}^* |j_{AB}\rangle_{sub} \tag{A.25}$$

so that

$$\sum_{i=1}^{2} |w_i\rangle_{sub}\langle w_i|_{sub} = \sum_{j=1}^{2} |j_{AB}\rangle_{sub}\langle j_{AB}|_{sub} = \rho_{AB}^{GHZ}. \tag{A.26}$$

Thus, it means that there is an another ensemble $\{r_i, |w_i\rangle\}$, where r_i is the weight of $|w_i\rangle$ in the ensemble, which represent the mixed state ρ_{AB}^{GHZ} such that

$$\rho_{AB}^{GHZ} = \sum_{i=1}^{2} r_i |w_i\rangle\langle w_i|. \tag{A.27}$$

Meanwhile, since $C(\rho_{AB}^{GHZ}) \geq 0$, then the density matrix ρ_{AB}^{GHZ} is of the first class which leads to consider the following procedure to find the optimal ensemble.

Begin with the general decomposition defined by Eq. (A.25) for the subnormalized states $\{|w_i\rangle\}$ of ρ_{AB}^{GHZ} where the unitary matrix is chosen to diagonalize the Hermitian matrix $\tau\tau^*$ with the eigenvalues square of the absolute values of the eigenvalues of the R matrix. In the same sense, it is sufficient to determine the eigenvectors $|t_i\rangle$ of the $\tau\tau^*$ which construct the columns of $U^\dagger$.

The matrix elements τ_{ij} of τ are formed by *"tilde inner products"*:

$$\tau_{ij} = \langle i_{AB} | \widetilde{j_{AB}} \rangle \tag{A.28}$$

where $| \widetilde{j_{AB}} \rangle$ is the spin flipped state of the eigenstate $|j_{AB}\rangle$ of ρ_{AB}^{GHZ} defined by $| \widetilde{j_{AB}} \rangle = \sigma_y^{\otimes 2} \left| j_{AB}^* \right\rangle$ by means of the Pauli-Y operator $\sigma_y^{\otimes 2} = \sigma_y \otimes \sigma_y$ acting separately on each qubit such that

$$| \widetilde{j_{AB}} \rangle = \frac{\left(\mu_j - \| |a_2\rangle \|^2\right) |\tilde{a}_1\rangle + \langle a_1 | a_2 \rangle |\tilde{a}_2\rangle}{\sqrt{\pm \sqrt{\triangle} \left(\mu_j - \| |a_2\rangle \|^2\right)}} \tag{A.29}$$

or simply

$$| \widetilde{j_{AB}} \rangle = d_i \left(m_i |\tilde{a}_1\rangle + n |\tilde{a}_2\rangle\right). \tag{A.30}$$

Since, the eigenvalues $\lambda_i^2 = \gamma_i$ of $\tau\tau^*$ are known, it is possible to find the eigenvectors $|t_i\rangle$ of $\tau\tau^*$ corresponding to them by the eigenvector-eigenvalue relation:

$$(\tau\tau^* - \gamma_i I) |t_i\rangle = 0 \tag{A.31}$$

or equivalently in matrix notation

$$\begin{pmatrix} (\tau\tau^*)_{11} - \gamma_i & (\tau\tau^*)_{12} \\ (\tau\tau^*)_{21} & (\tau\tau^*)_{22} - \gamma_i \end{pmatrix} \begin{pmatrix} e_i \\ f_i \end{pmatrix} = 0 \tag{A.32}$$

where $(\tau\tau^*)_{ij}$'s are the matrix element of $\tau\tau^*$; e_i and f_i are the vector elements of $|t_i\rangle$ which can be chosen as $e_i = (\tau\tau^*)_{12}$ and $f_i = \gamma_i - (\tau\tau^*)_{11}$ then $|t_i\rangle$ can be written

$$|t_i\rangle = \frac{1}{t_i} \begin{pmatrix} (\tau\tau^*)_{12} \\ \gamma_i - (\tau\tau^*)_{11} \end{pmatrix} = g_i \begin{pmatrix} (\tau\tau^*)_{12} \\ \gamma_i - (\tau\tau^*)_{11} \end{pmatrix} \tag{A.33}$$

with the normalization constant t_i defined by $t_i = g_i^{-1} = \sqrt{|e_i|^2 + |f_i|^2}$. Therefore, the unitary matrix U can be written as

$$U = \begin{pmatrix} \langle t_1 | \\ \langle t_2 | \end{pmatrix} = \begin{pmatrix} g_1 (\tau^*\tau)_{12} & g_1 [\gamma_1 - (\tau^*\tau)_{11}] \\ g_2 (\tau^*\tau)_{12} & g_2 [\gamma_2 - (\tau^*\tau)_{11}] \end{pmatrix}. \tag{A.34}$$

By means of the complex conjugate of the unitary matrix U^*

$$U^* = \begin{pmatrix} \langle t_1^* | \\ \langle t_2^* | \end{pmatrix} = \begin{pmatrix} g_1 (\tau\tau^*)_{12} & g_1 [\gamma_1 - (\tau\tau^*)_{11}] \\ g_2 (\tau\tau^*)_{12} & g_2 [\gamma_2 - (\tau\tau^*)_{11}] \end{pmatrix}, \tag{A.35}$$

the subnormalized states $|w_i\rangle_{sub}$ can be formed as

$$|w_i\rangle_{sub} = \sum_{j=1}^{2} U_{ij}^* |j_{AB}\rangle = g_i \left\{ (\tau\tau^*)_{12} |1_{AB}\rangle + [\gamma_i - (\tau\tau^*)_{11}] |2_{AB}\rangle \right\} \tag{A.36}$$

and or in terms of $\{|a_i\rangle\}$

$$\begin{aligned} |w_i\rangle_{sub} &= g_i \{(d_1 m_1 (\tau\tau^*)_{12} + d_2 m_2 \gamma_i - d_2 m_2 (\tau\tau^*)_{11}) |a_1\rangle \\ &\quad + n^* [d_2 \gamma_i + (\tau\tau^*)_{12} - (\tau\tau^*)_{11}] |a_2\rangle\} \end{aligned} \tag{A.37}$$

or simply

$$|w_i\rangle_{sub} = w_{i1} |a_1\rangle + w_{i2} |a_2\rangle \tag{A.38}$$

where

$$w_{i1} = g_i [m_2 \gamma_i + m_1 (\tau\tau^*)_{12} - m_2 (\tau\tau^*)_{11}] \tag{A.39}$$

and

$$w_{i2} = \frac{n^*}{g_i} [\gamma_i + (\tau\tau^*)_{12} - (\tau\tau^*)_{11}] . \tag{A.40}$$

Then construct

$$(\tau\tau^*)_{11} = \tau_{11}\tau^*_{11} + \tau_{21}\tau^*_{21}, \tag{A.41}$$

$$(\tau\tau^*)_{12} = \tau_{11}\tau^*_{12} + \tau_{12}\tau^*_{22}, \tag{A.42}$$

$$(\tau\tau^*)_{12} - (\tau\tau^*)_{11} = \tau_{11} (\tau^*_{12} - \tau^*_{11}) + \tau_{12} (\tau^*_{22} - \tau^*_{21}) \tag{A.43}$$

put them into

$$m_1 (\tau\tau^*)_{12} - m_2 (\tau\tau^*)_{11} = \tau_{11} (m_1 \tau^*_{12} - m_2 \tau^*_{11}) + \tau_{12} (m_1 \tau^*_{22} - m_2 \tau^*_{21}) \tag{A.44}$$

to obtain $\{|w_i\rangle_{sub}\}$.

If one can find anything about $\{|w_i\rangle_{sub}\}$ after the above calculations, next s/he has to find the second set of states $\{|y_i\rangle\}$ and finally, if it is possible, it is time to find the real orthogonal matrix V transforming the second set $\{|y_i\rangle\}$ to the optimal set $\{|z_i\rangle\}$. Therefore, it is better to apply the new method to those type examples (see Sec. 3.2).