

Characterization of Multipartite Entanglement

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Abstract

In this thesis, we discuss several aspects of the characterization of entanglement in multipartite quantum systems, including detection, classification and quantification of entanglement. First, we discuss triqubit pure entanglement and propose a special true tripartite entanglement, the mixed entanglement, besides the Greenberger-Horne-Zeilinger (GHZ) entanglement and the W entanglement. Then, based on quantitative complementarity relations, we draw entanglement Venn diagrams for triqubit pure states with different entanglements and introduce the total tangle $\tau^{(T)}$ to quantify total entanglement of triqubit pure states by defining the union I that is equivalent to the total tangle $\tau^{(T)}$ from the mathematical point of view. The generalizations of entanglement Venn diagrams and the union I to N -qubit pure states are also discussed. Finally, based on the ranks of reduced density matrices, we discuss the separability of multiparticle arbitrary-dimensional pure and mixed states, respectively.

Chapter 1

Introduction

Entanglement plays an important role not only in quantum mechanics but also in quantum information theory (See, e.g., Refs. [1–8]). It is one of the remarkable features that distinguishes quantum mechanics from classical mechanics. The word “Entanglement” was first coined by Erwin Schrödinger in 1935 [9].

Entanglement refers to quantum correlations between spatially-separated physical systems that can be stronger than correlations allowed by classical mechanics. It is this property of entanglement which caused that Einstein, Podolsky and Rosen published a famous paper in 1935 [10] now celebrated as EPR paper in which they raised fundamental questions about the completeness of quantum mechanics. In the EPR paper, Einstein and his coauthors constructed a wonderful scenario where one can immediately precisely predict the result of a measurement on one part of a system by measuring on another part of the system even though the two parts are spatially separated by a distance $\geq c(t - t_0)$ (where c is the speed of the light and t and t_0 are the final and initial time, respectively, when one puts the two parts of the system in two different points.) after they have interacted with each other. This is the so-called EPR paradox. Following this scenario, Einstein and his coauthors concluded that quantum theory must be incomplete if the locality were to be respected.

In the same year as the EPR paper appeared, Schrödinger introduced the concept of entanglement in the paper “Present situation in quantum mechanics” [9] for reacting to Einstein, Podolsky and Rosen’s criticism [10]. Schrödinger also introduced his famous cat (now called Schrödinger’s cat) as an extreme illustration of entanglement. In this model, a cat and a decaying atom, which are connected by a trigger and a vial of cyanide, are in a definite entangled state. If the atom were to decay and trigger the release of cyanide, the cat would die; otherwise the cat would live. The system composed of

the decaying atom and the cat whose situation is unknown is in a typical entangled state. The quantum mechanical description of the system is a coherent superposition of one state in which the atom is still excited and the cat is alive, and other state in which the atom has decayed and the cat is dead. The state of the coherent superposition can be written as:

$$\frac{1}{\sqrt{2}}(|\text{excited, alive}\rangle + |\text{decayed, dead}\rangle) \quad (1.1)$$

After three decades from the EPR paradox and the Schrödinger's cat, Bell made an essential progress on the debate of entanglement in 1964. In the paper "On the Einstein-Podolsky-Rosen paradox" [11], Bell derived correlation inequalities now called Bell's inequalities, which can be violated in quantum mechanics but have to be satisfied within every model that is local and complete, the so-called local hidden-variable models. By Bell's outstanding contribution, it became possible to experimentally test whether the local hidden-variable models can explain all observed physical phenomena.

Up to now, many experiments [12] on violations of Bell inequalities have been reported. These experiments obviously invalidated the local hidden-variable models and supported the quantum-mechanical view of nature. In particular, the violation of Bell's inequalities demonstrates the presence of entanglement in quantum systems.

In 1989, Werner [13] introduced an important family of biqubit mixed states, which are now called Werner states. Werner states do not violate any Bell inequalities though they can be entangled states.

Thus, from the quantum mechanical point of view, we are still too far from understanding entanglement, a counterintuitive quantum phenomenon that lies at the heart of modern quantum theory.

On the other side, the attitude towards entanglement has been changed in the last two decades from it being focused on the fundamental applications of quantum mechanics (See, e.g., [1, 3, 4, 6–8]), i.e., quantum information theory including quantum computation and quantum communication.

In 1982, Feynman [14] suggested to use quantum systems to simulate complicated quantum systems, a very hard task in the classical computer. In 1985, Deutsch [15] proposed the first algorithms based on the laws of quantum mechanics. Deutsch's algorithms, which found the field of quantum computation, could solve certain tasks faster than any classical computer. In 1994, Shor [16] discovered a polynomial-time quantum algorithm, which tremendously saves computation time, for factorizing prime numbers of a large integer. In 1997, Grover [17] proposed the search algorithm in quantum systems. In 2001, Raussendorf and Briegel [18] introduced the one-way computer in which entanglement lies at the core of the quantum computation.

In parallel, the applications of entanglement in quantum communication were developed. In 1984, Bennett and Brassard [19] proposed the first protocol in quantum cryptography, which is now called BB84 protocol and founded the field of quantum cryptography. In 1991, Ekert [20] proposed the first protocol for secret key distribution via entangled states. In 1992, Bennett and Wiesner [21] introduced the scheme of quantum dense coding. In 1993, Bennett and his coauthors [22] proposed the scheme of quantum teleportation. These two schemes and Shor's breakthrough generated an avalanche of interest in quantum information theory.

In experimental respect, much progress has been made in the last decade. For example, Deutsch's algorithm has been realized in an ion trap [23], Shor's algorithm has been implemented via nuclear magnetic resonance technique [24], quantum teleportation has been experimentally realized via photons [25], and so on. An extensive list of achievements can be found in Refs. [1, 4–6, 8].

Today, researchers treat entanglement not only as the heart of modern quantum mechanics but also as a fundamental resource of quantum information theory [8]. Thus it is of great importance to characterize entanglement qualitatively and quantitatively in quantum mechanics and quantum information theory (See, e.g., [1, 4, 5, 26–29]).

In this thesis, we will discuss the several aspects of characterizing entanglement in multipartite quantum systems via different tools in different cases. The thesis is organized as follows:

In chapter 2, we introduce the basic concepts and notations needed for the understanding of the rest of the thesis. We give simple introductions on several basic concepts in quantum mechanics and quantum information theory, such as Hilbert space, qubit and density matrix. Then we give the definition of entanglement in cases of pure and mixed states. Finally, we introduce the present situation of characterizing entanglement, including detecting, classifying and quantifying entanglement, which form the basis of our study.

In chapter 3, we discuss triqubit pure states and propose a special true tripartite entanglement, the mixed entanglement, which possesses the main properties of the the Greenberger-Horne-Zeilinger (GHZ) entanglement [30] and the W entanglement [31], simultaneously. Based on all linear combinations of up to five basis vectors of triqubit pure states [32], we find that there exist two inequivalent kinds of sets of four non-superfluous basis vectors for mixed entanglement.

In chapter 4, we draw entanglement Venn diagrams for triqubit pure states with different entanglements based on quantitative complementarity relations [33–35]. Following them, we define the union I , invoking an analogy

to set theory [36], for triqubit pure states. This allows us to introduce a new quantity, named the total tangle $\tau^{(T)}$, for quantifying the total entanglement of triqubit pure states. In fact, the union I and the total tangle $\tau^{(T)}$ are equivalent to each other from the mathematical point of view. Then we generalize the definition of the union I to N -qubit pure states and obtain interesting bounds to the union I with different entanglements. We also discuss an entanglement Venn diagram and the detailed formulation of the union I (and the total tangle $\tau^{(T)}$) for N -qubit pure states in conjecture.

In chapter 5, we focus on multiparticle arbitrary-dimensional states based on the ranks of the (reduced) density matrices. We derive two necessary and sufficient conditions for entangled and fully entangled pure states. Then we derive necessary conditions for the separability of mixed states, which are equivalent to sufficient conditions for entanglement.

The conclusion and outlook form the final chapter.

Chapter 2

Characterization of Entanglement

As mentioned in Chapter 1, it is of great importance to characterize entanglement in quantum mechanics and quantum information theory. In this chapter, we will focus on this subject and give an introduction on the main notations and concepts that will be used in the following chapters.

In the field of characterizing entanglement, there exist three main tasks, which can be described as three questions as follows:

- (1). “Is a state entangled at all?”
- (2). “How does a state entangle?”
- (3). “How much entanglement does a state possess?”

These three questions are stronger and stronger one by one on understanding entanglement and can be considered to be a three-step subject on studying entanglement.

For example, consider a multipartite state. The first step is to detect entanglement of the state, i.e., to answer the first question. That is, one would have the criterion to distinguish the entangled state from the separable state. The second step is to classify entanglement of the state, i.e., to answer the second question. That is, if the state is entangled, one would determine the means that the state entangles. The third step is to quantify entanglement of the state, i.e., to answer the third question. That is, one needs the measure to quantitatively characterize entanglement of the state.

Much progress on characterization of entanglement with different degree in different cases has been made (see the reviews, e.g., in Ref. [5, 8, 26–29] and the references therein.), in particular, in the last decade. However, all of these three questions are essentially open up to now (see, e.g., in Ref. [26–29]). Since the number of articles about entanglement has enormously increased during the last decade (for example, after the search with the key word

“entanglement ” in website “<http://www.arxiv.org/archive/quant-ph>”, a lot of results will be found.), it is almost impossible to give a complete overview on this subject, and this is not the purpose of this chapter. We will rather introduce some main and necessary concepts and notations on characterizing entanglement that will be used in the following chapters. Of course, some significant progress and fundamental work will be introduced even though they have no direct relation with the work of this thesis.

This chapter is organized as follows: In section 1, we introduce several basic concepts in quantum mechanics and quantum information theory. Then we give the definition of entanglement of pure and mixed states. Finally, we discuss the three tasks of characterization of entanglement in three sections, respectively.

2.1 Several basic concepts

In this section, we introduce several basic concepts in quantum mechanics and quantum information theory, such as, Hilbert space, qubit and density matrix.

2.1.1 Hilbert space

Hilbert space, an infinite dimensional vector space usually denoted as \mathcal{H} , is a mathematical framework suitable for describing the concepts, systems, principles, processes and laws of quantum mechanics. Formulating quantum mechanics in terms of Hilbert spaces, first introduced by von Neumann, was one of the most important steps in the development of modern quantum physics. Thus it is necessary to give some introduction on Hilbert space (also see, e.g., in Ref. [1–3]).

Hilbert space \mathcal{H} as a special kind of complex vector space has the following basic properties. Note that we will use Dirac’s notation to express vectors. A complex column vector $\vec{\psi}$ is expressed by a ket vector $|\psi\rangle$. The corresponding row vector is expressed by a bra vector $\langle\psi|$.

(1). Linearity: If two vectors $|u\rangle, |v\rangle \in \mathcal{H}$, for $\alpha, \beta \in \mathbb{C}$ (Here the symbol “ \mathbb{C} ” denotes the set of complex numbers), then

$$\alpha|u\rangle + \beta|v\rangle \in \mathcal{H}. \quad (2.1)$$

In particular, Hilbert space \mathcal{H} contains a null element, $\mathbf{0}$, such that

$$|u\rangle + \mathbf{0} = |u\rangle \quad (2.2)$$

for any $|u\rangle \in \mathcal{H}$.

(2). Inner product and norm: The inner product of a pair of vectors $|u\rangle$ and $|v\rangle$ corresponds to a complex number as

$$\langle v|u\rangle = \langle u|v\rangle^* = \sum_{i=1}^{\mathcal{D}} v_i^* u_i \quad (2.3)$$

where the symbol “ \mathcal{D} ” is the dimension of the vector.

The norm of vector $|u\rangle$, also called the length of vector, is defined as

$$\|u\| \equiv \sqrt{\langle u|u\rangle} \geq 0, \quad (2.4)$$

with the equality if and only if $|u\rangle = 0$.

(3). Completeness: Any strongly convergent sequence of elements $|u_n\rangle$ for $n \rightarrow \infty$ has a limit $|u\rangle$ and the limit $|u\rangle$ is also an element of \mathcal{H} . That is, there is a unique element $|u\rangle \in \mathcal{H}$ such that

$$\|u_n - u\|_{n \rightarrow \infty} \rightarrow 0. \quad (2.5)$$

Now we will discuss several important concepts of Hilbert space as follows.

(1). Dimension of Hilbert space: The dimension of a finite dimensional Hilbert space \mathcal{H} is defined as the maximal number of linear independent vectors of \mathcal{H} . A d -dimensional Hilbert space will be denoted as \mathcal{H}_d .

(2). Orthogonality: Two vectors $|u\rangle, |v\rangle \in \mathcal{H}$ are called orthogonal if

$$\langle u|v\rangle = \langle v|u\rangle = 0. \quad (2.6)$$

A set $U \subseteq \mathcal{H}$ is orthogonal if any two of its elements are orthogonal and all its elements have norm 1. Orthogonal states (represented by orthogonal vectors) are states that are independent of each other.

The importance of orthogonality in quantum mechanics is that whenever a measurement is performed on a quantum system, if those quantum states are mutually orthogonal, then the measurement can obtain distinguishable outcomes. Otherwise no measurement can distinguish faithfully between non-orthogonal states.

(3). Tensor product: Consider two vectors $|u\rangle$ and $|v\rangle$ as

$$\begin{aligned} |u\rangle &= (u_1, u_2, \dots, u_m)^T \in \mathcal{H}_{|u\rangle}, \\ |v\rangle &= (v_1, v_2, \dots, v_n)^T \in \mathcal{H}_{|v\rangle}, \end{aligned} \quad (2.7)$$

where the superscript “ T ” means the transpose of the vector. The tensor product of $|u\rangle$ and $|v\rangle$, denoted as $|u\rangle \otimes |v\rangle$, is an $(m * n)$ -dimensional vector of Hilbert space \mathcal{H} with elements

$$\begin{aligned} |u\rangle \otimes |v\rangle &= (u_1|v\rangle, u_2|v\rangle, \dots, u_m|v\rangle)^T \\ &= (u_1v_1, u_1v_2, \dots, u_1v_n, u_2v_1, \dots, u_mv_n)^T. \end{aligned} \quad (2.8)$$

Here the $(m * n)$ -dimensional Hilbert space \mathcal{H} is the so-called tensor product of $\mathcal{H}_{|u\rangle}$ and $\mathcal{H}_{|v\rangle}$ which is written as

$$\mathcal{H} = \mathcal{H}_{|u\rangle} \otimes \mathcal{H}_{|v\rangle}. \quad (2.9)$$

2.1.2 Qubit

One of the fundamental concept of classical information theory is the bit, which takes one of the two possible values $\{0, 1\}$. The corresponding concept of the bit in quantum information theory is called the quantum bit, or qubit [37] for short. It describes a state in the simplest possible quantum system.

Consider a two-dimensional Hilbert space \mathcal{H} , the smallest nontrivial Hilbert space. Two basis vectors for the Hilbert space \mathcal{H} are denoted in the following way:

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} = |0\rangle \quad \text{and} \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |1\rangle. \quad (2.10)$$

Then a qubit is defined as a quantum state

$$|\psi\rangle \equiv \alpha|0\rangle + \beta|1\rangle \quad (2.11)$$

where α, β are complex numbers that satisfy $|\alpha|^2 + |\beta|^2 = 1$, and the overall phase is physically irrelevant. Put another way, the state of a qubit is a unit vector in a two-dimensional complex vector space. The special states $|0\rangle$ and $|1\rangle$ form an orthonormal basis for this vector space.

We can perform a measurement that projects the qubit onto the basis $\{|0\rangle, |1\rangle\}$. Then we will obtain the outcome $|0\rangle$ with probability $|\alpha|^2$, and the outcome $|1\rangle$ with probability $|\beta|^2$. Furthermore, except in the case $\alpha = 0$ and $\beta = 0$, the measurement irrevocably disturbs the state of the qubit. After the measurement, the qubit has been prepared in a known state (either $|0\rangle$ or $|1\rangle$) that differs (in general) from its initial state. If the value of the qubit is originally unknown, there is no way to determine α and β with the single projected measurement, or any other conceivable measurement. For the classical bit, we can measure it without disturbing, and we can decipher all of the information that it encodes. Thus the essential difference between the classical bit and the qubit is that a classical bit has a state either 0 or 1 with the corresponding probabilities, while a qubit can be in a state other than $|0\rangle$ or $|1\rangle$. That is, a qubit can be in a state linearly combined by two basis vectors $|0\rangle$ and $|1\rangle$, which is the so-called superposition, a basic difference of quantum world from classical world.

The ability of a qubit to be in a superposition state runs counter to our “common sense” understanding of the physical world around us. As pointed

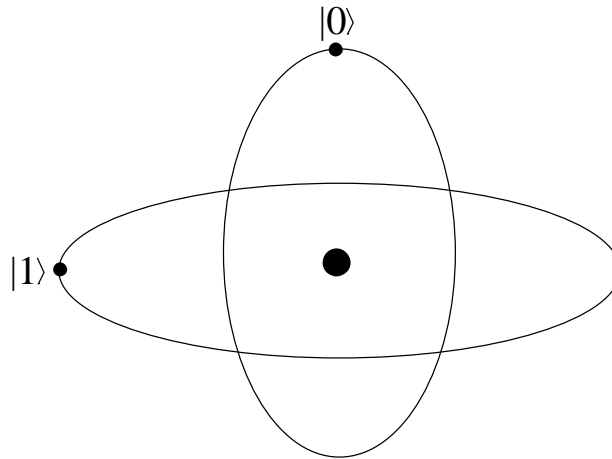


Figure 2.1: Qubit represented by two electronic levels in an atom.

out, a classical bit is in a state either 0 or 1. By contrast, a qubit can exist in a continuum of states between $|0\rangle$ and $|1\rangle$.

By the definition of the qubit in Eq. (2.11), any two-state quantum system can be called a qubit when the two states span a two-dimensional Hilbert space. This is more general, and the interpretation is more difficult. Therefore, any two-state quantum system is a potential candidate for a qubit, such as, the photon with two different polarizations, the nuclear spin with different alignments in a uniform magnetic field, the single atom orbited by an electron with two different states as shown in Fig. (2.1), and so on.

2.1.3 Density matrix

Similar to the state vector as the language to formulate quantum mechanics, the density matrix is known as an alternate tool to describe quantum systems. The alternate formulation of quantum mechanics by the density matrix language extends mathematically the state vector approach, since it provides a much more convenient means for thinking about quantum systems whose states are not completely known, for example, mixed states.

Consider a quantum system which is in one of a number of pure states $\{|\psi_i\rangle\}$ with respective probabilities p_i . We can call $\{|\psi_i\rangle, p_i\}$ an ensemble of pure states, or a mixed state. The density matrix of this mixed state is defined as

$$\rho \equiv \sum_i p_i |\psi_i\rangle \langle \psi_i|. \quad (2.12)$$

If any one of the probabilities is equal to 1 while all the others are 0, then

this definition of the density matrix in Eq. (2.12) is reduced to the case of the pure state $|\psi\rangle$ as

$$\rho = |\psi\rangle\langle\psi|. \quad (2.13)$$

Thus the definition of the density matrix in Eq. (2.12) can also be rewritten as

$$\rho \equiv \sum_i p_i \rho^i \quad (2.14)$$

where $\rho^i = |\psi_i\rangle\langle\psi_i|$. It turns out immediately that all the formulation of quantum mechanics can be re-expressed in terms of the density matrix language.

From the definition of the density matrix in Eqs. (2.12) and (2.13), we can obtain the following properties of density matrix ρ (the proofs of these properties are omitted):

- (1) ρ is self-adjoint (hermitian), i.e.,

$$\rho = \rho^\dagger \quad (2.15)$$

where “ ρ^\dagger ” denotes the conjugate transposed matrix of ρ .

- (2) ρ has trace equal to 1, i.e.,

$$\text{Tr}(\rho) = 1. \quad (2.16)$$

- (3) ρ is positive definite, i.e.,

$$\rho \geq 0. \quad (2.17)$$

- (4) The inequality

$$\text{Tr}(\rho^2) \leq 1 \quad (2.18)$$

holds, with equality if and only if ρ is a pure state. Then we easily get a necessary and sufficient condition for a pure state as

$$\rho^2 = \rho \quad (2.19)$$

holds if and only if ρ is pure. From these properties we directly obtain that ρ can be diagonalized, that the eigenvalues are all real and nonnegative, and that the eigenvalues sum to one.

When considering a composite quantum system in terms of the density matrix, the reduced density matrix is a necessary tool for describing subsystems. Consider a composite system ρ_{AB} of two systems A and B . The reduced density matrix ρ_A for system A is defined as

$$\rho_A \equiv \text{Tr}_B(\rho_{AB}) \quad (2.20)$$

where Tr_B is a map of operators known as the partial trace over system B . The partial trace is defined as

$$\begin{aligned}\text{Tr}_B(|a_1\rangle\langle a_2| \otimes |b_1\rangle\langle b_2|) &\equiv |a_1\rangle\langle a_2|\text{Tr}(|b_1\rangle\langle b_2|) \\ &= |a_1\rangle\langle a_2|\langle b_2|b_1\rangle\end{aligned}\quad (2.21)$$

where $|a_1\rangle$ and $|a_2\rangle$ are any two vectors on the state space of A , and $|b_1\rangle$ and $|b_2\rangle$ are any two vectors in the state space of B .

The reduced density matrix ρ_A provides the correct measurement statistics for measurements made on system A . For example, consider one of the Bell states

$$|\Psi\rangle_{AB} = \frac{1}{\sqrt{2}}(|0_A1_B\rangle + |1_A0_B\rangle) \quad (2.22)$$

Then

$$\begin{aligned}\rho_{AB} &= |\Psi\rangle_{AB}\langle\Psi| = \frac{1}{2}(|01\rangle\langle 01| + |01\rangle\langle 10| + |10\rangle\langle 01| + |10\rangle\langle 10|) \\ &= \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\end{aligned}\quad (2.23)$$

Tracing over qubit B , we obtain the reduced density matrix ρ_A as:

$$\begin{aligned}\rho_A &= \text{Tr}_B\rho_{AB} = \frac{1}{2}\text{Tr}_B(|01\rangle\langle 01| + |01\rangle\langle 10| + |10\rangle\langle 01| + |10\rangle\langle 10|) \\ &= \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\end{aligned}\quad (2.24)$$

It is the maximally mixed state.

2.2 Definition of entanglement

“What is entanglement?”

From the different starting points of research, physicists can give different answers for this question. Here we will discuss this question in two different cases of pure and mixed states, respectively, from the quantum mechanical and quantum informational points of view.

2.2.1 Pure states

In 1935, Schrödinger [9] gave the first qualitative definition of entanglement as

If two separable bodies, each by itself known maximally, enter a situation in which they influence each other, and separate again, then there occurs regularly that which I have (just) called entanglement of our knowledge of the two bodies.

About the “strange” property of entanglement, he wrote

For an entangled state, “the best possible knowledge of the whole does not include the best possible knowledge of its parts”. Thus “The whole is in a definite state, the parts taken individually are not”.

This explanation is now understood as the essence of entanglement of pure states.

In mathematical terms, entanglement of pure states is defined as: A pure state ρ of N particles A_1, A_2, \dots, A_N is called entangled when it can NOT be written as

$$\rho = \rho_{A_1} \otimes \rho_{A_2} \otimes \dots \otimes \rho_{A_N} = \bigotimes_{i=1}^N \rho_{A_i} \quad (2.25)$$

where ρ_{A_i} is the single-particle reduced density matrix given by $\rho_{A_i} \equiv \text{Tr}_{\{A_j\}}(\rho)$ for $\{A_j | \text{all } A_j \neq A_i\}$. Otherwise the state is separable.

Let us consider the simplest case: a state $|\Psi\rangle_{AB}$ of two qubits A and B , which are associated with two Hilbert spaces \mathcal{H}_A and \mathcal{H}_B , respectively. Then state $|\Psi\rangle_{AB}$ is associated with Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ whose elements include the tensor products of the elements in two subspaces \mathcal{H}_A and \mathcal{H}_B , such as $|0_A 0_B\rangle$, $|0_A 1_B\rangle$, $|1_A 0_B\rangle$ and $|1_A 1_B\rangle$. Because of the superposition of quantum systems, any linear combinations of these four product states could be possible, for example,

$$|\psi\rangle_{AB} = \alpha|00\rangle + \beta|11\rangle \in \mathcal{H}. \quad (2.26)$$

This state, which is called entangled state, cannot be described as the tensor product of two states $|a\rangle \in \mathcal{H}_A$ and $|b\rangle \in \mathcal{H}_B$. That is, there is no pair of vectors $|a\rangle \in \mathcal{H}_A$ and $|b\rangle \in \mathcal{H}_B$ such that $|\psi\rangle_{AB} = |a, b\rangle$. Thus, the existence of entangled states is a direct consequence of the tensor product structure of the Hilbert space describing composite quantum systems.

The most important property of entangled states is that they carry quantum correlations, which are quite different from classical correlations. The classical correlations are strictly restricted by Bell’s inequalities [11], whereas the quantum correlations corresponding to entangled states may violate them.

This is why with the correlations contained in entangled states we can perform things that are impossible using classical correlations.

In order to create entangled states out of product states, we need interactions. If we do not have interactions, the Hamiltonian \hat{H} describing the evolution of systems A and B will be written as

$$\hat{H} = \hat{H}_A \otimes \hat{I}_B + \hat{I}_A \otimes \hat{H}_B \quad (2.27)$$

where \hat{H}_A (\hat{H}_B) is the Hamiltonian of system A (B) and \hat{I} is the identity (unit) matrix. Since $\hat{H}_A \otimes \hat{I}_B$ and $\hat{I}_A \otimes \hat{H}_B$ commute with each other, we have the unitary evolution operator $\hat{U}(t)$ acting on the composite system, which can be always written as

$$\hat{U}(t) = \hat{U}_A(t) \otimes \hat{U}_B(t) \quad (2.28)$$

where $\hat{U}_A(t)$ ($\hat{U}_B(t)$) is the evolution operator acting on the system A (B). The product state $|\psi(0)\rangle_{AB} = |a(0)\rangle \otimes |b(0)\rangle$ will evolve into

$$\begin{aligned} |\psi(t)\rangle_{AB} &= (\hat{U}_A(t)|a(0)\rangle) \otimes (\hat{U}_B(t)|b(0)\rangle) \\ &= |a(t)\rangle \otimes |b(t)\rangle \end{aligned} \quad (2.29)$$

which is still a product state. Operators with the form (2.28) are called local operators. Thus one says that entanglement cannot be created by local operators (even with the help of classical communication).

2.2.2 Mixed states

The definition of entanglement of mixed states is more complex than the one of pure states. In general, we would like to use the description introduced by Werner in [13] as

A state is called entangled if it cannot be prepared by local operations (and classical communication) out of a product state.

From this description, we directly get that entanglement can only be produced by interactions.

In mathematical terms, the definition of entanglement of mixed states is given as: A mixed state ρ of N particles A_1, A_2, \dots, A_N , described by M probabilities p_j and M pure states ρ^j as $\rho = \sum_{j=1}^M p_j \rho^j$, is called entangled when it can NOT be written as

$$\rho = \sum_{j=1}^M p_j \bigotimes_{i=1}^N \rho_{A_i}^j \quad (2.30)$$

where $p_j > 0$ for $j = 1, 2, \dots, M$ with $\sum_{j=1}^M p_j = 1$.

2.3 Detection of entanglement

“Is a state entangled at all?”

At present, it is one of the hot fields in the characterization of entanglement to find the criterion on the separability of quantum systems. Though it is still an open question on detection of entanglement (see, e.g., [26–29]), much progress has been made in the last few years (see, e.g., [38–41], and the references in the reviews [28, 29, 42]). Here we will simply introduce some basic concepts and significant results.

In general, the criteria on the separability of quantum states can be separated into operational entanglement criteria and non-operational entanglement criteria. Here the word “operational” is used to emphasize, as pointed out by Bruß [27], that an operational criterion can be applied to an explicit density matrix ρ , giving some immediate answer like “ ρ is separable,” or “ ρ is entangled,” or “this criterion is not strong enough to decide whether ρ is separable or entangled.”

2.3.1 Operational criteria

First, we will introduce some operational entanglement criteria, such as, the Schmidt decomposition, the partial transposition criterion, the reduction criterion and the majorization criterion.

(1). Schmidt decomposition [2, 43]: Any bipartite pure state $|\psi\rangle_{AB} \in \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ can be decomposed, by choosing an appropriate basis, as

$$|\psi\rangle_{AB} = \sum_{i=1}^m \alpha_i |a_i\rangle \otimes |b_i\rangle \quad (2.31)$$

where $1 \leq m \leq \min\{\dim(\mathcal{H}_A), \dim(\mathcal{H}_B)\}$, and $\alpha_i > 0$ with $\sum_{i=1}^m \alpha_i^2 = 1$. Here $|a_i\rangle$ ($|b_i\rangle$) form a part of an orthonormal basis in \mathcal{H}_A (\mathcal{H}_B). The positive numbers α_i are called the Schmidt coefficients of $|\psi\rangle_{AB}$ and the number m is called the Schmidt rank of $|\psi\rangle_{AB}$.

If the Schmidt decomposition of a bipartite pure state has more than one Schmidt coefficient, the state is entangled. Unfortunately, there is no general Schmidt decomposition for any N -partite pure state until now though we can generalize the Schmidt decomposition to more than 2 subsystems [44], for example, the generalized Schmidt decomposition to triqubit pure states has been proposed in [32].

However, for an N -partite quantum system in a pure state, it is possible to detect the separability of the system with respect to all partitions of N subsystems into 2 parts. If the system with respect to at least one partition

of 2 parts is entangled as detected by the bipartite Schmidt decomposition, the N -partite state is entangled. Of course, this method is quite fussy since one has to check all partitions of 2 parts. (This is why we propose a way to study the separability of a pure state based on the ranks of the reduced density matrices in Chapter 5.)

(2). Partial transpose criterion [45]: The partial transpose of a composite density matrix is given by transposing only one of the subsystems. For example, consider ρ of two subsystems A and B , the partially transposed matrix ρ^{TA} with respect to subsystem A is given by

$$(\rho^{TA})_{m\mu,n\nu} = \rho_{n\mu,m\nu} \quad (2.32)$$

where the Latin indices, which have been transposed, are referring to subsystem A and the Greek indices to subsystem B .

Then the partial transpose criterion can be described as:

If a state ρ_{AB} is separable, then

$$\rho_{AB}^{TA} \geq 0 \quad \text{and} \quad \rho_{AB}^{TB} \geq 0 \quad (2.33)$$

hold.

It has been shown [46] that the positivity of the partial transpose is a necessary and sufficient condition for the separability only for composite states of dimension 2×2 and 2×3 , while it is only a necessary condition for higher dimensions.

(3). Reduction Criterion [47]: If a state ρ_{AB} is separable, then

$$\rho_A \otimes \hat{I}_B - \rho_{AB} \geq 0 \quad \text{and} \quad \hat{I}_A \otimes \rho_B - \rho_{AB} \geq 0 \quad (2.34)$$

hold.

Similar to the partial transpose criterion, the reduction criterion is a necessary and sufficient condition only for dimensions 2×2 and 2×3 , and a necessary condition in other cases.

(4). Majorization Criterion [48]: If a bipartite state ρ_{AB} is separable, then

$$\lambda_{\rho_{AB}}^\downarrow \prec \lambda_{\rho_A}^\downarrow \quad \text{and} \quad \lambda_{\rho_{AB}}^\downarrow \prec \lambda_{\rho_B}^\downarrow \quad (2.35)$$

have to be fulfilled. Here λ_ρ^\downarrow denotes the vector consisting of the eigenvalues of ρ , in decreasing order, and a vector x^\downarrow is majorized by a vector y^\downarrow , denoted as $x^\downarrow \prec y^\downarrow$, when $\sum_{i=1}^k x_i^\downarrow \leq \sum_{i=1}^k y_i^\downarrow$ holds for $k = 1, \dots, (d-1)$, and the equality holds for $k = d$, with d being the dimension of the vector. Zeros are appended to the vectors $\lambda_{\rho_A}^\downarrow$ and $\lambda_{\rho_B}^\downarrow$ in (2.35), in order to make their dimensions equal to the one of $\lambda_{\rho_{AB}}^\downarrow$.

The majorization criterion is only a necessary, not a sufficient condition for separability.

2.3.2 Non-operational criteria

Here, we will introduce two non-operational entanglement criteria, the positive maps and the entanglement witness.

(1). Positive maps [46]: Denoting the set of operators acting on Hilbert space \mathcal{H}_1 by $\hat{\mathcal{O}}_1$, and the set of operators acting on Hilbert space \mathcal{H}_2 by $\hat{\mathcal{O}}_2$. The operators $\hat{\mathcal{O}}_1$ (/or $\hat{\mathcal{O}}_2$) constitute a Hilbert space (the so-called Hilbert-Schmidt space) denoted by $\mathcal{H}\{\hat{\mathcal{O}}_1\}$ (/or $\mathcal{H}\{\hat{\mathcal{O}}_2\}$). The space of the linear maps from $\hat{\mathcal{O}}_1$ onto $\hat{\mathcal{O}}_2$ is denoted by $\mathcal{L}(\hat{\mathcal{O}}_1, \hat{\mathcal{O}}_2)$. A linear Hermitian map $\Lambda \in \mathcal{L}(\hat{\mathcal{O}}_1, \hat{\mathcal{O}}_2)$ is a transformation denoted as

$$\Lambda(\hat{\mathcal{O}}_1) \rightarrow \hat{\mathcal{O}}_2, \quad (2.36)$$

which

(i). is linear, i.e.,

$$\Lambda(\alpha\hat{A} + \beta\hat{B}) = \alpha\Lambda(\hat{A}) + \beta\Lambda(\hat{B}) \quad (2.37)$$

for any operator $\hat{A}, \hat{B} \in \hat{\mathcal{O}}_1$, and α, β are complex numbers;

(ii). maps Hermitian operators onto Hermitian operators, i.e.,

$$\Lambda(\hat{A}) = \Lambda(\hat{A}^\dagger) = (\Lambda(\hat{A}))^\dagger \quad (2.38)$$

for any operator $\hat{A} \in \hat{\mathcal{O}}_1$.

A linear Hermitian map $\Lambda \in \mathcal{L}(\hat{\mathcal{O}}_1, \hat{\mathcal{O}}_2)$ is a positive map if it maps positive operators in $\hat{\mathcal{O}}_1$ onto positive operators in $\hat{\mathcal{O}}_2$, i.e., for $\hat{A} \in \hat{\mathcal{O}}_1$,

$$\hat{A} \geq 0 \implies \Lambda(\hat{A}) \geq 0. \quad (2.39)$$

A positive map $\Lambda \in \mathcal{L}(\hat{\mathcal{O}}_1, \hat{\mathcal{O}}_2)$ is completely positive if for any tensor extension Λ' of the form

$$\Lambda' = \hat{I} \otimes \Lambda \quad (2.40)$$

where

$$\Lambda'(M_n \otimes \hat{A}) \rightarrow M_n \otimes \Lambda(\hat{A}), \quad (2.41)$$

Λ' is positive for all n , where $\hat{A} \in \hat{\mathcal{O}}_1$, M_n stands for the set of the complex matrices with dimension $n \times n$, and \hat{I} here denotes the identity map on Hilbert space $\mathcal{H}(M_n)$.

Then the positive map criterion can be described as:

A state ρ is separable if and only if for any positive map Λ ,

$$(\hat{I} \otimes \Lambda)\rho \geq 0 \quad (2.42)$$

holds.

(2). Entanglement witness [46, 49]: A state ρ is entangled if and only if there exists a Hermitian operator \hat{W} such that

$$\text{Tr}(\hat{W}\rho) < 0, \quad (2.43)$$

and for any separable state ρ_{sep}

$$\text{Tr}(\hat{W}\rho_{sep}) \geq 0. \quad (2.44)$$

Since violation of Bell's inequalities is a manifestation of quantum entanglement, a natural separability criterion is constituted by Bell's inequalities. Werner [13] first pointed out that separable states must satisfy all possible Bell's inequalities. However, Bell's inequalities are only necessary, not sufficient conditions for separability. In fact, Bell's inequalities are essentially a special type of the entanglement witness.

Although both criteria, the positive map and the entanglement witness, are necessary and sufficient for any bipartite system, they do not provide us with a simple and operational procedure to check the separability of a given state. Therefore the study of operational necessary and sufficient criteria on separability of quantum systems is still a very hot field in quantum information theory and quantum mechanics.

2.4 Classification of entanglement

“How does a state entangle?”

In fact, we can separate this question into two questions, i.e., to convert the task of classifying entanglement into a two-step task. The first question focuses on “how many subsystems in a multipartite state are indeed entangled?” For example, triqubit pure states can be roughly classified into three types, (fully) separable states, biseparable states and fully (true tripartite) entangled states (We will discuss them in detail). Then for the entangled states with the same number of entangled subsystems (exactly speaking, with respect to the same partition of subsystem), we focus on the equivalence classes of entanglement in different states [50–52]. For example, by means of local operations and classical communication (LOCC) with nonzero probability, i.e., stochastic LOCC (SLOCC) [52], there are two different kinds of full (true tripartite) entanglement in triqubit pure states [31]. Any triqubit fully entangled pure state can be converted into one of two standard forms, namely either the GHZ state [30]

$$|\text{GHZ}\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle), \quad (2.45)$$

or the W state

$$|W\rangle = \frac{1}{\sqrt{3}}(|001\rangle + |010\rangle + |100\rangle). \quad (2.46)$$

Many methods of classification of entanglement (see, e.g., [31, 32, 38, 51, 53–61]) have been proposed in the last few years. Here we will introduce several important methods.

2.4.1 Hierarchic classification

Based on the separability properties of certain partitions of systems into subsystems, Dür *et al.* [55, 56] proposed a complete, hierarchic classification of a family of states, where the states, which have the same number of particles and the corresponding particles have the same Hilbert-space dimensions, are put into different levels of a hierarchy with respect to their entanglement properties.

Let us introduce the concept of k -separable states with N ($N \geq k$) particles [56]. A pure state ρ of N particles A_1, A_2, \dots, A_N is called k -separable with respect to a special partition into k parts if and only if ρ can be written as

$$\rho = \rho_1 \otimes \rho_2 \otimes \dots \otimes \rho_k = \bigotimes_{j=1}^k \rho_j \quad (2.47)$$

where ρ_j is the density matrix of the j -th part in the partition. This definition can be directly generalized to the mixed state. A mixed state ρ , where $\rho = \sum_{i=1}^M p_i \rho^i$, is k -separable if and only if it can be written as

$$\rho = \sum_{i=1}^M p_i \rho_1^i \otimes \rho_2^i \otimes \dots \otimes \rho_k^i = \sum_{i=1}^M p_i \bigotimes_{j=1}^k \rho_j^i. \quad (2.48)$$

The basic idea of the hierarchic classification is to consider all possible partitions of k parts for all k ($k \in \{2, 3, \dots, N\}$) and detect for each partition whether the given state is k -separable or not. The procedure is divided into levels, starting with $k = N$ (level N), continuing with $k = N - 1$ (level $(N - 1)$), \dots , until $k = 2$ (level 2). At each level k , we have all possible partitions of k -separability and (or) k -inseparability. The different levels of this structure are not independent of each other.

Consider two levels l and k , and suppose $l < k$. If a partition P_l of l parts can be obtained from a partition P_k of k parts by joining some of the parts of P_k , then we say that P_k is contained in P_l . On one hand, each partition of k parts is contained in various partitions of l parts, while on the other

hand, a number of different partitions of k parts can be contained in the same partition of l parts.

l -separability with respect to all partitions of l parts, which contain a certain partition P_k of k parts, is a necessary but not sufficient condition for k -separability with respect to partition P_k . k -separability with respect to a certain partition P_k of k parts implies l -separability with respect to all partitions of l parts which contain the partition P_k . Therefore, k -separability partly fixes the structure at lower levels l ($l < k$), while l -inseparability fixes some properties at higher levels k . The hierarchic classification is constructed in this way. Two states belong to the same separability class if they are separable with respect to the same partition.

However, Bennett *et al.* proposed a kind of triqubit mixed states in [62]. In those states, the entanglement across any partition into 2 parts is zero, but the state is entangled. That is, for a triqubit system separability with respect to all partitions into 2 parts is not sufficient to guarantee 3-separability (i.e., full separability when considering each qubit as a separated part) of the system.

2.4.2 Classifying triqubit mixed states

The Schmidt decomposition is a very good tool to study entanglement of bipartite pure states. The Schmidt number provides an important variable to classify entanglement. For example, using Schmidt numbers of a multiparticle pure state with respect to all possible partitions of the particles into 2 parts, we can roughly classify this state, though it is very complex for calculation.

For the further classification, we need the generalized Schmidt decomposition. Though the general Schmidt decomposition for an N -qubit state is unknown until now, a generalized Schmidt decomposition for triqubit pure states [32] has been proposed so that the classification of triqubit pure states is possible.

Another important method to classify entanglement is by local operations and classical communication (LOCC) [51, 52]. Reversible local operations among multipartite quantum systems are used to define equivalent classes in the set of entangled states. Here the equivalent classes of entangled states are said to contain the same kind of entanglement. This method leads to a celebrated result that all kinds of biqubit entanglement are equivalent to the Einstein-Podolsky-Rosen (EPR) entanglement [50].

By this method, Dür *et al.* [31] classified entanglement of triqubit pure states ρ_{ABC} into six inequivalent classes as:

- Fully separable states with the form $\rho_{ABC} = \rho_A \otimes \rho_B \otimes \rho_C$. This class of entanglement can be denoted as $A - B - C$.
- Biseparable states including three inequivalent classes as:
 1. Biseparable states with the form $\rho_{ABC} = \rho_A \otimes \rho_{BC}$. This class is denoted as $A - BC$.
 2. Biseparable states with the form $\rho_{ABC} = \rho_B \otimes \rho_{AC}$. This class is denoted as $B - AC$.
 3. Biseparable states with the form $\rho_{ABC} = \rho_C \otimes \rho_{AB}$. This class is denoted as $C - AB$.
- Fully (true tripartite) entangled states including two inequivalent classes as:
 1. The GHZ class represented by the GHZ state.
 2. The W class represented by the W state.

The classification of triqubit pure states will be discussed in Chapter 3 in detail. Here we will focus on the case of triqubit mixed states.

Since any triqubit mixed state can be decomposed as convex combination of pure states, triqubit mixed states can be classified by generalizing the classification of pure states [58]. To this aim, Acín *et al.* defined the following classes:

- Class S of separable states, i.e., those that can be expressed as a convex sum of projectors onto product vectors.
- Class B of biseparable states, i.e., those that can be expressed as a convex sum of projectors onto product and bipartite entangled vectors ($A - BC$, $B - AC$ and $C - AB$).
- Class W of the W state, i.e., those that can be expressed as a convex sum of projectors onto product, biseparable, and W-type vectors.
- Class GHZ of the GHZ state, i.e., the set of all physical states.

All these sets are convex and compact, and satisfy the relation

$$S \subset B \subset W \subset \text{GHZ}. \quad (2.49)$$

States in the class S are not entangled. Only for the production of states belonging to the classes W and GHZ , true tripartite entanglement is needed.

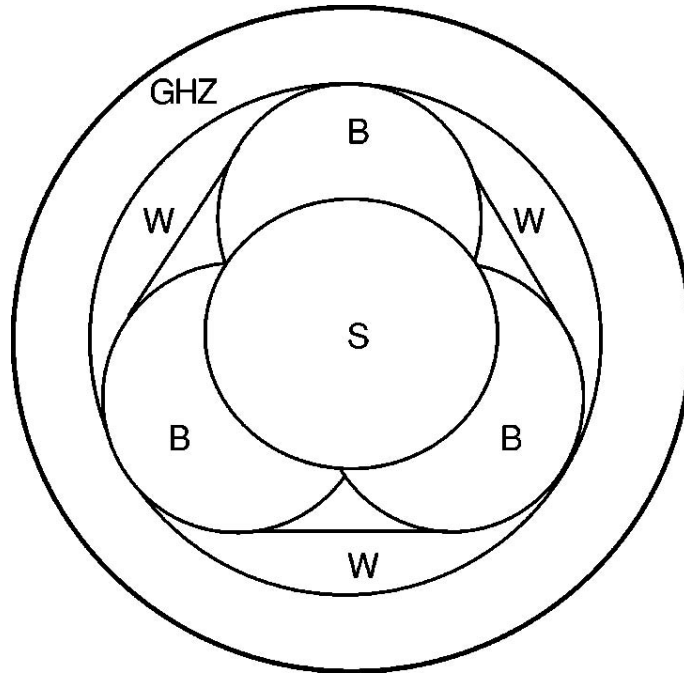


Figure 2.2: (from [58]) Schematic structure of the set of all triqubit states. S : separable class; B : biseparable class (convex hull of biseparable states with respect to any partition); W class and GHZ class.

The formation of entangled states in the subset $W|B$ requires W -type vectors with true tripartite entanglement, but zero 3-way entanglement. Finally, the class GHZ contains all types of entanglement, and in particular, GHZ -type vectors are required to prepare states from the subset $GHZ|W$. These classes are schematically shown by Acín *et al.* [58] in Fig. (2.2).

The classification of entangled states of higher dimensions is still under intensive research (see, e.g., Refs. [63–67]).

2.5 Quantification of entanglement

“How much entanglement does a state possess?”

Since there are many different kinds of entanglement, it is almost impossible to find a general measure for all kinds of entanglement. Even for the same kind of entanglement, there are several different measures with different aspects. For example, we have measures such as von Neumann entropy, relative entropy, concurrence, and so on, to quantify entanglement in biqubit pure states. Therefore many measures of entanglement have been introduced

in the last decade, for example, the relative entropy of entanglement [68, 69], the negativity [70], the robustness of entanglement [71, 72], the distillable entanglement [51, 73], the entanglement of formation [51], the entanglement cost [51, 74], the Schmidt measure [75], the universal measure of entanglement [76], and other measures (see the references of the reviews, e.g., [77, 78]). Among them, one of the most important measures of entanglement is the entanglement of formation. There have been several entanglement measures which are related with the entanglement of formation, such as, the concurrence [79, 80], the I -concurrence [81, 82], the n -tangle [83, 84], and so on. However, the quantification of entanglement is perhaps the most challenging open problem of modern quantum theory so far. We will give a simple introduction on this topic.

2.5.1 Requirements for measures

Here we will list several conditions for a quantity E to be a good measure of entanglement [68, 85, 86]. However, it is still an open question whether all these conditions are indeed necessary (also sufficient) for a quantity to be a good entanglement measure. In fact, some of the entanglement measures are useful for practical application but they do not fulfill all the conditions that will be listed.

(1). Normalization: Measure E vanishes on separable states and takes its maximum on maximally entangled states. The normalization of the entanglement measure can be considered as two conditions, which are expressed as:

(1-a). A state ρ is separable if and only if

$$E(\rho) = 0 \tag{2.50}$$

holds.

(1-b). The entanglement of a maximally entangled state ρ_M^d of two d -dimensional systems is given by

$$E(\rho_M^d) = \log_2 d. \tag{2.51}$$

(2). No increase under LOCC: Measure E of state ρ cannot increase under any LOCC operation Λ_{LOCC} , i.e.,

$$E(\Lambda_{LOCC}(\rho)) \leq E(\rho). \tag{2.52}$$

(2-a). Local unitary invariance: Measure E of state ρ is invariant under any local unitary \hat{U} , i.e.,

$$E(\hat{U}\rho\hat{U}^*) = E(\rho). \tag{2.53}$$

(3). Convexity: Measure E should be a convex function, i.e.,

$$E(\lambda\rho + (1 - \lambda)\sigma) \leq \lambda E(\rho) + (1 - \lambda)E(\sigma) \quad (2.54)$$

for any two states ρ and σ , and $0 \leq \lambda \leq 1$.

(4). Continuity: In the limit of vanishing distance between two density matrices ρ and σ , the difference between their entanglements should tend to zero, i.e.,

$$|E(\rho) - E(\sigma)| \rightarrow 0 \quad (2.55)$$

for $\|\rho - \sigma\| \rightarrow 0$.

(5). Additivity: A certain number n of identical copies of the state ρ should contain n times the entanglement of one copy, i.e.,

$$E(\rho^{\otimes n}) = nE(\rho). \quad (2.56)$$

(6). Subadditivity: The entanglement of the tensor product of two states ρ and σ should not be greater than the sum of the entanglements of each of the states, i.e.,

$$E(\rho \otimes \sigma) \leq E(\rho) + E(\sigma). \quad (2.57)$$

2.5.2 Several important measures

Here we introduce the concepts of several important entanglement measures. Some of them are necessary for the work in this thesis.

von Neumann entropy $E_S(\rho_{AB})$ (see, e.g., [1]): For a bipartite pure state ρ_{AB} , a good entanglement measure is the von Neumann entropy of its reduced density matrices as

$$E_S(\rho_{AB}) = S(\rho_A) = S(\rho_B) \quad (2.58)$$

where

$$S(\rho) = -\text{Tr}(\rho \log_2 \rho). \quad (2.59)$$

We will discuss von Neumann entropy in detail in chapter 4.

Relative entropy $S(\rho||\sigma)$: The relative entropy $S(\rho||\sigma)$ of ρ to its closest separable state σ is defined as

$$\begin{aligned} S(\rho||\sigma) &\equiv \text{Tr}(\rho(\log_2 \rho - \log_2 \sigma)) \\ &= \text{Tr}(\rho \log_2 \rho) - \text{Tr}(\rho \log_2 \sigma). \end{aligned} \quad (2.60)$$

Thus the relative entropy $S(\rho||\sigma)$ can be seen intuitively as the “distance” of the entangled state ρ to its closest separable state σ , although it is not a distance in the mathematical sense.

Here the closest separable state σ of a given state ρ is defined as the separable state that realizes the minimum of Eq. (2.60).

Distillable entanglement $E_D(\rho)$: The distillable entanglement $E_D(\rho)$ is defined as, roughly speaking, the asymptotic ratio with which maximally entangled states ρ_M can be distilled at most out of state ρ , i.e.,

$$E_D(\rho) \equiv \sup_{\{\Lambda_{LOCC}\}} \lim_{n \rightarrow \infty} \frac{n_{\rho_M}^{\text{out}}}{n_{\rho}^{\text{in}}} \quad (2.61)$$

where the supremum is taken over all possible distillation protocols via LOCC operations. Thus $E_D(\rho)$ tells us how much entanglement we can extract from a given state ρ , i.e., what is the ratio of the number of maximally entangled states ρ_M over the needed input state ρ , maximized over all possible distillation protocols.

Entanglement of formation $E_F(\rho)$: Any state ρ can be decomposed as a convex combination of pure states ρ^i , i.e., $\rho = \sum_i p_i \rho^i$. The entanglement of formation $E_F(\rho)$ is defined as the averaged von Neumann entropy of the reduced density matrices of ρ^i , minimized over all possible decompositions, i.e.,

$$E_F(\rho) \equiv \inf_{\rho = \sum_i p_i \rho^i} \sum_i p_i E_S(\rho^i) \quad (2.62)$$

where the infimum is taken over all possible decompositions of ρ . Thus $E_F(\rho)$ is intended to quantify the resources needed to create an entangled state ρ .

The variational problem that defines $E_F(\rho)$ is extremely difficult to solve [87]. However, some solutions for qubit and bipartite systems are known [80, 81], and some related entanglement measures have been introduced [83, 84]. We will discuss them in detail in the following part.

Entanglement cost $E_C(\rho)$: The entanglement cost $E_C(\rho)$ is defined as the asymptotic ratio of the number of maximally entangled input states ρ_M over the produced output entangled states ρ , minimized over all possible LOCC operations, i.e.,

$$E_C(\rho) \equiv \inf_{\{\Lambda_{LOCC}\}} \lim_{n \rightarrow \infty} \frac{n_{\rho_M}^{\text{in}}}{n_{\rho}^{\text{out}}} \quad (2.63)$$

where the infimum is taken over all possible LOCC operations. $E_C(\rho)$ tell us how expensive it is to create an entangled state ρ .

The distillable entanglement $E_D(\rho)$ and the entanglement cost $E_C(\rho)$ have been shown to be lower and upper bounds for any entanglement measure $E(\rho)$, respectively, i.e., [88]

$$E_D(\rho) \leq E(\rho) \leq E_C(\rho). \quad (2.64)$$

It is also conjectured that the entanglement of formation $E_F(\rho)$ and the entanglement cost $E_C(\rho)$ are identical, i.e., [51]

$$E_F(\rho) \stackrel{?}{=} E_C(\rho). \quad (2.65)$$

2.5.3 Concurrence and 3-tangle

Concurrence, which is related to the entanglement of formation, perhaps is the most important entanglement measure for qubit states. Here we will introduce the concurrence and some measures proposed following the concurrence.

The concurrence \mathcal{C}_{AB} of a qubit state ρ_{AB} is defined as follows [80]. For a given qubit state ρ_{AB} , the ‘‘spin-flipped’’ density matrix $\tilde{\rho}_{AB}$ is introduced as

$$\tilde{\rho}_{AB} = (\sigma_y \otimes \sigma_y) \rho_{AB}^* (\sigma_y \otimes \sigma_y) \quad (2.66)$$

where ρ_{AB}^* denotes the complex conjugated matrix of ρ_{AB} in the basis vectors $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$, and σ_y , one of Pauli matrices, in the same basis vectors, is given by

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \quad (2.67)$$

As both ρ_{AB} and $\tilde{\rho}_{AB}$ are positive operators, it follows that the product $(\rho_{AB} \tilde{\rho}_{AB})$, though non-Hermitian, also has only real and non-negative eigenvalues. Let the square roots of the these eigenvalues, in decreasing order, be denoted as $\lambda_1, \lambda_2, \lambda_3$ and λ_4 . Then the concurrence \mathcal{C}_{AB} of ρ_{AB} is defined as

$$\mathcal{C}_{AB} \equiv \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}. \quad (2.68)$$

For the special case in which ρ_{AB} is pure, the concurrence \mathcal{C}_{AB} can also be written as

$$\mathcal{C}_{AB} = 2\sqrt{\det(\rho_A)} = 2\sqrt{\det(\rho_B)} \quad (2.69)$$

where ρ_A (ρ_B) is the reduced density matrix of ρ_{AB} , and $\det(\rho)$, defined as $\det(\rho) \equiv |\rho|$, denotes the determinant of matrix ρ . It can be shown that $\mathcal{C}_{AB} = 0$ corresponds to a separable state, $\mathcal{C}_{AB} = 1$ corresponds to the maximally entangled state, such as, the Bell states.

Then the entanglement of formation $E_F(\rho_{AB})$ is given by

$$E_F(\rho_{AB}) = h\left(\frac{1 + \sqrt{1 - \mathcal{C}_{AB}^2}}{2}\right) \quad (2.70)$$

where $h(x)$ is the binary entropy function as

$$h(x) = -x \log_2 x - (1 - x) \log_2(1 - x). \quad (2.71)$$

Similar to some papers (see, e.g., Ref. [83, 84] and [89–91] in which the squared concurrence is applied to measure entanglement of quantum states) after Wootters introduced the detailed formulation of the concurrence, we would rather take the squared concurrence as the measure for entanglement of two qubits in this thesis.

The generalization of the concurrence for a bipartite arbitrary-dimensional state ρ_{AB} has been proposed by Rungta *et al.* with the name *I*-concurrence [81, 82]. The *I*-concurrence $\mathcal{C}^{(I)}(\rho_{AB})$ for a pure state ρ_{AB} of a $d_A \times d_B$ system is simply related to the purity of the marginal density matrices as [81]

$$\mathcal{C}^{(I)}(\rho_{AB}) \equiv \sqrt{2(1 - \text{Tr}(\rho_A^2))} \equiv \sqrt{2(1 - \text{Tr}(\rho_B^2))} \quad (2.72)$$

This definition is given in terms of the universal-inverter superoperator [81], which has been shown to be a natural generalization to higher dimensions of the spin flip for qubits.

Following the definition of the entanglement of formation, the *I*-concurrence is extended to the mixed state ρ_{AB} by the convex roof as

$$\mathcal{C}^{(I)}(\rho_{AB}) \equiv \inf_{\{p_i, \rho^i\}} \left(\sum_i p_i \mathcal{C}^{(I)}(\rho^i) \right) \quad (2.73)$$

where $\rho_{AB} = \sum_i p_i \rho^i$ for pure states ρ^i and the infimum is taken over all possible decompositions of ρ_{AB} .

Relating with the Wootters' definition of the concurrence for biqubit states, Coffman, Kundu and Wootters [83] proposed an entanglement measure, named the 3-tangle, for quantifying 3-way entanglement in triqubit pure states. Note that *n*-way entanglement [84] is one type of multiparticle entanglement which critically involves all *n* particles and has the property that tracing out any one or several ones of the *n* particles leaves the remaining particles unentangled. For example, consider the GHZ state, in which, after tracing out any one of the three qubits, the other two qubits are separable [92]. Therefore the entanglement of the GHZ state is also called 3-way entanglement, which is quite different from the entanglement of the W state. (We will discuss them in detail in chapter 3.) For biqubit entangled states, it is obvious from the definitions that 2-way entanglement is the same as bipartite entanglement.

The 3-tangle, denoted as τ , of a triqubit pure state ρ_{ABC} is defined as

$$\tau = \mathcal{C}_{i(jk)}^2 - \mathcal{C}_{ij}^2 - \mathcal{C}_{ik}^2 \quad (2.74)$$

for $i, j, k \in \{A, B, C\}$. Here $\mathcal{C}_{i(jk)}^2$ denotes the squared concurrence between qubit *i* and pair of qubits (*jk*). After a detailed mathematical derivation [83],

the 3-tangle τ is written as

$$\tau = 4|d_1 - 2d_2 + 4d_3| \quad (2.75)$$

where

$$\begin{cases} d_1 = a_{000}^2 a_{111}^2 + a_{100}^2 a_{011}^2 + a_{010}^2 a_{101}^2 + a_{001}^2 a_{110}^2, \\ d_2 = a_{000} a_{111} a_{100} a_{011} + a_{000} a_{111} a_{010} a_{101} + a_{000} a_{111} a_{001} a_{110} \\ \quad + a_{100} a_{011} a_{010} a_{101} + a_{100} a_{011} a_{001} a_{110} + a_{010} a_{101} a_{001} a_{110}, \\ d_3 = a_{000} a_{011} a_{101} a_{110} + a_{111} a_{100} a_{010} a_{001}. \end{cases} \quad (2.76)$$

Here, for example, a_{000} denotes the coefficient of the basis vector $|000\rangle$ in the wave function $|\psi\rangle_{ABC}$ of state ρ_{ABC} with $\rho_{ABC} = |\psi\rangle_{ABC} \langle\psi|$, where

$$|\psi\rangle_{ABC} = \sum_{i,j,k} a_{ijk} |ijk\rangle \quad (2.77)$$

for $i, j, k \in \{0, 1\}$. In a more standard form of algebra, τ can be rewritten as

$$\tau = 2 \left| \sum a_{ijk} a_{i'j'm} a_{npk'} a_{n'p'm'} \epsilon_{ii'} \epsilon_{jj'} \epsilon_{kk'} \epsilon_{mm'} \epsilon_{nn'} \epsilon_{pp'} \right| \quad (2.78)$$

where the sum is over all the indices, and

$$\begin{cases} \epsilon_{00} = \epsilon_{11} = 0, \\ \epsilon_{01} = -\epsilon_{10} = 1. \end{cases} \quad (2.79)$$

Recently, Lee, Joo and Kim [93] proposed an entanglement measure, named the partial tangle, to represent the residual two-qubit entanglement in a triqubit pure state.

The partial tangle, denoted as τ_{ij} , of a triqubit pure state ρ_{ABC} is defined as

$$\tau_{ij} \equiv \sqrt{\mathcal{C}_{i(jk)}^2 - \mathcal{C}_{ik}^2} = \sqrt{\mathcal{C}_{ij}^2 + \tau} \quad (2.80)$$

for $i, j \in \{A, B, C\}$. Thus we cannot say that τ_{ij} represents only the entanglement for two qubits in the composite system ρ_{ABC} since τ_{ij} is not equivalent to \mathcal{C}_{ij} in general as in Eq.(2.80).

In Ref. [84], Wong and Christensen proposed a potential measure named the n -tangle for quantifying the n -way entanglement of an n -qubit pure state. This n -tangle, denoted as $\tau_{1\dots n}$, is defined as

$$\tau_{1\dots n} \equiv 2 \left| \sum a_{\alpha_1 \dots \alpha_n} a_{\beta_1 \dots \beta_n} a_{\gamma_1 \dots \gamma_n} a_{\delta_1 \dots \delta_n} \right. \\ \left. \times \epsilon_{\alpha_1 \beta_1} \epsilon_{\alpha_2 \beta_2} \cdots \epsilon_{\alpha_{n-1} \beta_{n-1}} \epsilon_{\gamma_1 \delta_1} \epsilon_{\gamma_2 \delta_2} \cdots \epsilon_{\gamma_{n-1} \delta_{n-1}} \epsilon_{\alpha_n \gamma_n} \epsilon_{\beta_n \delta_n} \right| \quad (2.81)$$

for all even n and $n = 3$. Here the ϵ terms are given in Eq. (2.79). The a terms are the coefficients in the wave function $|\psi\rangle$ in terms of the basis vectors as

$$|\psi\rangle = \sum_{i_1 \cdots i_n} a_{i_1 \cdots i_n} |i_1 \cdots i_n\rangle. \quad (2.82)$$

However, this generalization of the 3-tangle causes some trouble as can be seen as follows. For example, consider the 4-qubit pure state $|\psi\rangle_{ABCD}$ that is the tensor product of two singlet states as

$$|\psi\rangle_{ABCD} = \frac{1}{\sqrt{2}}(|01\rangle_{AB} - |10\rangle_{AB}) \otimes \frac{1}{\sqrt{2}}(|01\rangle_{CD} - |10\rangle_{CD}). \quad (2.83)$$

It is obvious that there is no 4-way entanglement in state $|\psi\rangle_{ABCD}$, but a simple calculation shows that the 4-tangle defined in Eq.(2.81) has a value of 1 for this state.

Chapter 3

Mixed Entanglement in Triqubit Pure States

As mentioned in the preceding chapter, characterizing entanglement of arbitrary biqubit states, including detecting, classifying and quantify biqubit entanglement, has been well solved. On detecting biqubit entanglement, Peres [45] proposed a standard criterion to distinguish entangled biqubit states from separable states. Bennett *et al.* [50] have shown that there is only one class of biqubit entanglement, Bell entanglement, so that any biqubit pure state can be concentrated by local operations and classical communications into maximally entangled states such as the Bell states. Wootters and his colleagues [79, 80] proposed the concurrence, related with the entanglement of formation introduced by Bennett *et al.* in [51], as the measure of biqubit entanglement, which has been considered as the most important measure of biqubit entanglement now.

Now multipartite entanglement is still under intensive research. With the rapid development of quantum information theory (see, e.g., [1, 4–6]), for the simplest multipartite entanglement, triqubit entanglement, one contributes not only to whether a triqubit state is entangled or not but also to how it entangles and how much entanglement it possesses.

In this chapter, we will discuss triqubit pure entanglement and propose a special true tripartite entanglement, the mixed entanglement, for triqubit pure states. This chapter is organized as follows: In section 1, we discuss the present problem of classifying triqubit pure entanglement and give the motivation of our study. In section 2, we give some introductions on the GHZ entanglement and the W entanglement. In section 3, we propose the mixed entanglement in triqubit pure states and discuss it in detail. In the final section, with mixed entanglement, we discuss an interesting experiment reported by Walther, Resch and Zeilinger in Ref. [94] recently and reveal some

nature of entanglement changing in this experiment.

3.1 Motivation

On classifying entanglement of triqubit pure states, very many results have been obtained in the last few years (see, e.g., [31, 32, 57, 95–97, 112]). Among them, there are two significant results obtained by Acín *et al.* in [32] and Dür *et al.* in [31], respectively.

It has been proved that [99, 100] the number of entanglement parameters for any triqubit pure state is five and there exists a reference form in terms of six basis vectors for any triqubit pure state by using repeatedly the bipubit Schmidt decomposition. The five entanglement parameters are one phase (all others can be absorbed) and four moduli of the coefficients among the six basis vectors.

Then Acín *et al.* [32] proved that there exist three inequivalent sets of five basis vectors

$$\begin{aligned} & \{|000\rangle, |001\rangle, |010\rangle, |100\rangle, |111\rangle\}, \\ & \{|000\rangle, |001\rangle, |110\rangle, |100\rangle, |111\rangle\}, \\ & \{|000\rangle, |101\rangle, |110\rangle, |100\rangle, |111\rangle\}, \end{aligned} \quad (3.1)$$

so that any triqubit pure state can be written as a linear combination of the five basis vectors of one and the same set. That is, any triqubit pure entanglement is uniquely characterized by the five entanglement parameters. This is the so-called generalized Schmidt decomposition to triqubit pure states. Suppose to select the last set of sets (3.1), the generalized Schmidt decomposition can be written as

$$|\Psi\rangle = \lambda_1|000\rangle + \lambda_2|101\rangle + \lambda_3|110\rangle + \lambda_4 e^{i\varphi}|100\rangle + \lambda_5|111\rangle \quad (3.2)$$

where we have chosen the fourth coefficient to carry the only relevant phase and all $\lambda_i > 0$, $0 \leq \varphi \leq \pi$, $\sum_i \lambda_i^2 = 1$.

By defining a new quantity Δ as

$$\Delta = |\lambda_4 \lambda_5 e^{i\varphi} - \lambda_2 \lambda_3|^2, \quad (3.3)$$

Acín *et al.* introduced five J_i 's as

$$\begin{cases} J_1 \equiv \Delta, & \in [0, 1/4] \\ J_2 \equiv \lambda_1^2 \lambda_2^2, & \in [0, 1/4] \\ J_3 \equiv \lambda_1^2 \lambda_3^2, & \in [0, 1/4] \\ J_4 \equiv \lambda_1^2 \lambda_5^2, & \in [0, 1/4] \\ J_5 \equiv \lambda_1^2 (\Delta + \lambda_2^2 \lambda_3^2 - \lambda_4^2 \lambda_5^2). \end{cases} \quad (3.4)$$

The J_i 's are indicators of entanglement in some sense: J_1 (J_2, J_3) indicate bipartite entanglement, J_4 indicates GHZ entanglement, only when all of them vanish there is no entanglement at all. Therefore pure states of three qubits A, B and C can be classified into:

- Type 1 (product states or fully separable states): $J_i = 0$ for $i = 1, 2, 3, 4, 5$ but not all $\lambda_i = 0$ for $i = 1, 2, 3, 4, 5$. For example,

$$|\Psi\rangle = \lambda_2|101\rangle + \lambda_4 e^{i\varphi}|100\rangle. \quad (3.5)$$

- Type 2-a (biseparable states): $J_i = 0$ for $i = 1, 2, 3, 4, 5$ except J_1 (J_2, J_3) when qubit A (B, C) is separable from the other two qubits. For example,

$$|\Psi\rangle = \lambda_2|101\rangle + \lambda_3|110\rangle + \lambda_4 e^{i\varphi}|100\rangle. \quad (3.6)$$

- Type 2-b (generalized GHZ states): $J_i = 0$ for $i = 1, 2, 3, 5$ but $J_4 > 0$. State $|\Psi\rangle$ is written as

$$|\Psi\rangle = \lambda_1|000\rangle + \lambda_5|111\rangle. \quad (3.7)$$

- Type 3-a (tri-Bell states): $\lambda_4 = \lambda_5 = 0$. State $|\Psi\rangle$ is written as

$$|\Psi\rangle = \lambda_1|000\rangle + \lambda_2|101\rangle + \lambda_3|110\rangle. \quad (3.8)$$

- Type 3-b (extended GHZ states): two of the three λ 's $\{\lambda_2, \lambda_3, \lambda_4\}$ are equal to zero. One represented state $|\Psi\rangle$ is written as

$$|\Psi\rangle = \lambda_1|000\rangle + \lambda_2|101\rangle + \lambda_5|111\rangle. \quad (3.9)$$

- Type 4-a: $\lambda_5 = 0$. State $|\Psi\rangle$ is written as

$$|\Psi\rangle = \lambda_1|000\rangle + \lambda_2|101\rangle + \lambda_3|110\rangle + \lambda_4 e^{i\varphi}|100\rangle. \quad (3.10)$$

- Type 4-b: $\lambda_2 = 0$. State $|\Psi\rangle$ is written as

$$|\Psi\rangle = \lambda_1|000\rangle + \lambda_3|110\rangle + \lambda_4 e^{i\varphi}|100\rangle + \lambda_5|111\rangle. \quad (3.11)$$

- Type 4-c: $\lambda_4 = 0$. State $|\Psi\rangle$ is written as

$$|\Psi\rangle = \lambda_1|000\rangle + \lambda_2|101\rangle + \lambda_3|110\rangle + \lambda_5|111\rangle. \quad (3.12)$$

Reversible local transformations among multipartite quantum systems are used to study equivalence classes in the set of entangled states [51, 52]. If two states can be transformed into each other by means of local operations and classical communication (LOCC) with nonzero probability, then these two states have the same class of entanglement. By reversible local transformations, Dür *et al.* [31] showed that there are two different classes of true tripartite entanglement: the GHZ class, whose representative is the GHZ state [30]

$$|\text{GHZ}\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle), \quad (3.13)$$

and the W class, whose representative is the W state

$$|\text{W}\rangle = \frac{1}{\sqrt{3}}(|001\rangle + |010\rangle + |100\rangle). \quad (3.14)$$

It also has been shown [31, 57] that one can not exactly interconvert the GHZ state and the W state under any LOCC. Besides these two inequivalent classes of entanglement, there are four inequivalent classes of entanglement which have been listed in Chapter 2 as the fully separable class and three biseparable classes $A - BC$, $B - AC$ and $C - AB$.

Experimentally, the GHZ state of three photons [101, 102] and three Rydberg atoms [103] have been observed. The W state also has been experimentally realized via photons [104] and via trapped ions [105]. Recently, an interesting experiment has been reported by Walther *et al.* in [94] that the local conversion of GHZ states to approximate W states is realized based on local positive operator valued measures (POVMs) and classical communication.

But in the 11th reference of Ref. [31], Dür *et al.* pointed out that their results are not fully compatible with the results of Refs. [32, 57]. Recently, some triqubit pure states with peculiar entanglement have also been reported in [95–97, 112] from several different respects. Thus the question of classifying triqubit pure entanglement is still not completely solved. And the nature of the entanglement changing in Walther *et al.*'s experiment is also worth research.

3.2 GHZ entanglement and W entanglement

The GHZ state was first introduced by Greenberger, Horne and Zeilinger [30] for the debate about whether quantum mechanics is a complete theory or not, i.e., Einstein, Podolsky and Rosen's criticism proposed in the EPR paper [10]. It is well known that using biqubit entangled states to test Bell's inequality,

the conflict with local realism only arises for statistical predictions. Greenberger, Horne and Zeilinger showed that quantum-mechanical predictions for certain measurement results on triqubit entangled states are in conflict with local realism in cases where quantum theory makes definite, i.e., non-statistical, predictions. That is, the quantum-mechanical predictions of the GHZ state are in stronger conflict with local realism than the conflict of all biqubit entangled states (see, e.g., Ref. [4]).

Gisin and Bechmann-Pasquinucci have pointed out that one of the main properties of the GHZ entanglement is that it is very fragile under particle losses [92], which means if one of the three qubits is traced out, the remaining state is completely unentangled, i.e., separable. That is, for a state with GHZ entanglement, any reduced state obtained by tracing the original state over one of the three qubits retains no entanglement. Thus the GHZ entanglement also is called the 3-way entanglement [83] and is quantified by the 3-tangle τ . In triqubit pure states, GHZ entanglement exists for $\tau > 0$ and the maximal GHZ entanglement (in the GHZ state) for $\tau = 1$.

In the contrast to GHZ entanglement, one of the main properties of W entanglement is that it is robust under disposal of any one of the three qubits, which means that for a state with W entanglement, the remaining state is still entangled if any one of the three qubits is traced out. But there is no 3-way entanglement in states with W entanglement at all. That is, for a state with W entanglement, three reduced states obtained by tracing the original state over one of the three qubits retain bipartite entanglement while $\tau = 0$ always holds in the original state. Thus W entanglement is considered to be composed of three bipartite entanglements together.

Taking the squared concurrence as the measure of bipartite entanglement, we have the following criterion: a pure state ρ of three qubits A , B and C contains W entanglement if

$$\min\{\mathcal{C}_{AB}^2, \mathcal{C}_{AC}^2, \mathcal{C}_{BC}^2\} > 0 \quad (3.15)$$

holds. Dür *et al.* [31] introduced a measure for W entanglement, here denoted as E_W , as

$$E_W \equiv \mathcal{C}_{AB}^2 + \mathcal{C}_{AC}^2 + \mathcal{C}_{BC}^2 \quad (3.16)$$

when condition (3.15) holds; otherwise the W entanglement is always zero no matter that one or two of the three bipartite entanglements are greater than zero. The W entanglement E_W achieves its maximal value $4/3$ in the W state.

The common character of GHZ entanglement and W entanglement is that both are composed of the three qubits together. Therefore they are called true tripartite entanglement (sometimes also called full entanglement of three

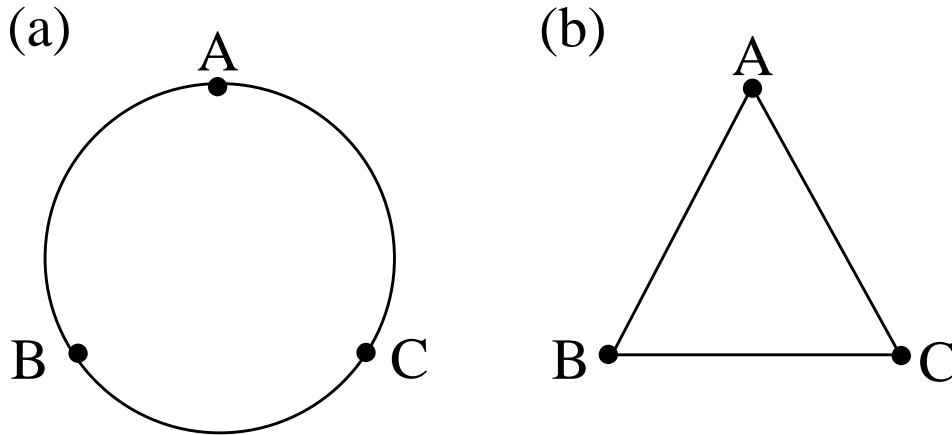


Figure 3.1: Diagrams for GHZ entanglement and W entanglement according to their different properties. The three dots in the diagrams denote three qubits A , B and C . In Diagram (a), the closed circle which connects the three qubits presents GHZ entanglement. If one of the three qubits is lost, i.e., if the circle is broken, GHZ entanglement would disappear and the remaining two qubits connected by the broken circle are not entangled with each other. Diagram (b) is for the W entanglement. Each short line which connects two qubits means the bipartite entanglement of the two qubits. It is obvious from Diagram (b) that the remaining two qubits connected by the short line are still entangled with each other after one of the three qubits is lost.

qubits). In Fig. (3.1), we draw different diagrams for GHZ entanglement and W entanglement according to their different properties.

3.3 Mixed entanglement

Without losing universality, suppose triqubit states are composed of three spin-1/2 particles. Denoting the state of a particle with spin z component $m = 1/2$ as $|0\rangle$ and the state with $m = -1/2$ as $|1\rangle$, then in the space of triqubit states, there are eight basis vectors shown in Table (3.1) with the total spin z component $\pm 3/2$ or $\pm 1/2$.

By the signs of the total spin z components, the eight basis vectors can be classified into two sets, the positive set of $|000\rangle$, $|001\rangle$, $|010\rangle$ and $|100\rangle$, and the negative set of the four remaining ones. By the number of particles with the same sign of the single spin z components in one and the same basis vector, the eight basis vectors can also be classified into two sets, the triple

Table 3.1: Classifications of eight basis vectors by the different relations of their spin z components.

	Triple	Double		
Positive	$ 000\rangle$	$ 001\rangle$	$ 010\rangle$	$ 100\rangle$
Negative	$ 111\rangle$	$ 110\rangle$	$ 101\rangle$	$ 011\rangle$

set of $|000\rangle$ and $|111\rangle$, and the double set of the remaining ones. According to the signs of the single spin z components of the corresponding particles in different basis vectors, the eight basis vectors can be separated into four complementary pairs as $|000\rangle$ and $|111\rangle$, $|001\rangle$ and $|110\rangle$, $|010\rangle$ and $|101\rangle$, $|100\rangle$ and $|011\rangle$, where the sum of the two total spin z components in a pair is equal to zero.

Now let us start the analysis of true tripartite entanglement in triqubit pure states based on all linear combinations of up to five basis vectors. We will take the squared concurrence and the 3-tangle as measures of 2- and 3-way entanglements, respectively.

States which are linear combinations of two basis vectors can only have GHZ entanglement for $\tau > 0$ as a form of true triqubit entanglement, and only when the two basis vectors are one of the four complementary pairs. These states are called generalized GHZ states in [32].

States which are linear combinations of three basis vectors can contain either GHZ entanglement or W entanglement. When states are combined of one of the four complementary pairs plus one of the remaining basis vectors, there is GHZ entanglement for $\tau > 0$ but no W entanglement since two of the three bipartite entanglements are zero. These states are called extended GHZ states in [32] and slice states in [57]. When states are combined of three basis vectors such as $|001\rangle$, $|010\rangle$ and $|100\rangle$, there is only W entanglement since condition (3.15) holds but no 3-way entanglement for $\tau = 0$. It is worth noting that [52] entanglement of states combined of $|001\rangle$, $|010\rangle$ and $|100\rangle$ is the same as that of states combined of $|101\rangle$, $|110\rangle$ and $|000\rangle$, which is called the tri-Bell states in [32], since these two states can be converted into each other by the spin-flip transformation of the first qubit.

States combined of four basis vectors can have a special true tripartite entanglement, the mixed entanglement, besides the GHZ entanglement and the W entanglement. For a state of three qubits A , B and C with mixed entanglement, on the one hand, there is 3-way entanglement, i.e., $\tau > 0$, in the state; on the other hand, three reduced density matrices ρ_{AB} , ρ_{AC}

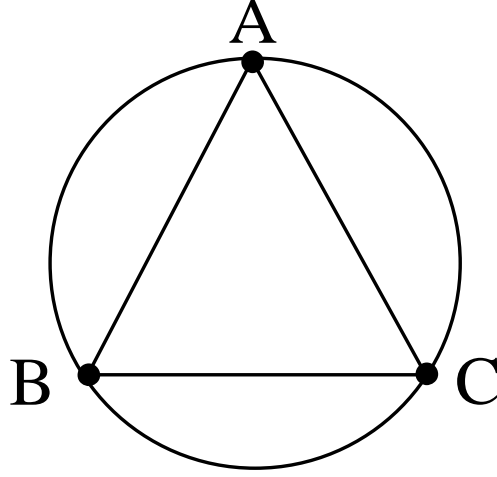


Figure 3.2: Diagram for the mixed entanglement. The dots in the diagram denote the qubits. The closed circle which connects the three qubits together represents the GHZ entanglement while three lines among the three qubits represent three bipartite entanglement, which together compose the W entanglement.

and ρ_{BC} all retain bipartite entanglement, i.e., condition (3.15) holds. The diagram of the mixed entanglement is drawn in Fig. (3.2). States with mixed entanglement can be constructed as linear combinations from two different kinds of sets of non-superfluous four basis vectors from Table (3.1) as explained below.

The first kind of the sets for combining states with mixed entanglement contains one of the four complementary pairs plus two of the remaining basis vectors in which the sum of the two total spin z components is ± 1 , for example,

$$\{|000\rangle, |001\rangle, |100\rangle, |111\rangle\}, \quad (3.17)$$

and a state based on this set can be written as

$$|\Psi\rangle = \lambda_1|000\rangle + \lambda_2|001\rangle + \lambda_3 e^{i\varphi}|100\rangle + \lambda_4|111\rangle \quad (3.18)$$

where the third coefficient is chosen to carry the only relevant phase and all $\lambda_i > 0$, $0 \leq \varphi \leq \pi$, $\sum_i \lambda_i^2 = 1$. Entanglement of this state is as follows

$$\begin{cases} \tau & = 4\lambda_1^2\lambda_4^2, \\ \mathcal{C}_{AB}^2 & = 4\lambda_2^2\lambda_3^2, \\ \mathcal{C}_{AC}^2 & = 4\lambda_2^2\lambda_4^2, \\ \mathcal{C}_{BC}^2 & = 4\lambda_3^2\lambda_4^2. \end{cases} \quad (3.19)$$

From Eqs. (3.19), it is apparent that there must be mixed entanglement in state (3.18) since all 2- and 3-way entanglements are greater than zero for all $\lambda_i > 0$.

In mixed entanglement of state (3.18), the GHZ entanglement relates only with the complementary pair $|000\rangle$ and $|111\rangle$, and the coefficients λ_2 and λ_3 of the two non-complementary basis vectors $|001\rangle$ and $|100\rangle$ do not contribute to the GHZ entanglement; while the W entanglement relates with three basis vectors $|001\rangle$, $|100\rangle$ and $|111\rangle$, the coefficient λ_1 of basis vector $|000\rangle$ does not contribute to the W entanglement. So basis vector $|111\rangle$ is the common basis vector of two different kinds of entanglement, GHZ entanglement and W entanglement.

In mixed entanglement based on the set (3.17) with all $\lambda_i > 0$ and $\sum_i \lambda_i^2 = 1$, GHZ entanglement τ from Eqs. (3.19) is strictly less than 1; it approaches that limiting value when λ_1 and λ_4 both approach $1/\sqrt{2}$. Similarly, W entanglement E_W is strictly less than $4/3$; it approaches that limiting value when λ_2 , λ_3 and λ_4 approach $1/\sqrt{3}$. That is, in mixed entanglement based on the set (3.17), τ and E_W are in the two open intervals as $\tau \in (0, 1)$ and $E_W \in (0, 4/3)$.

The second kind of the sets for combining states with mixed entanglement contains four basis vectors without the complementary pair in which the sum of the four total spin z components is zero, for example,

$$\{|001\rangle, |010\rangle, |100\rangle, |111\rangle\}, \quad (3.20)$$

and a state based on this set can be written as

$$|\Psi\rangle = \lambda_1|001\rangle + \lambda_2|010\rangle + \lambda_3 e^{i\varphi}|100\rangle + \lambda_4|111\rangle \quad (3.21)$$

where all $\lambda_i > 0$, $0 \leq \varphi \leq \pi$, and $\sum_i \lambda_i^2 = 1$. Its entanglement is as follows

$$\begin{cases} \tau & = 16\lambda_1\lambda_2\lambda_3\lambda_4, \\ \mathcal{C}_{AB}^2 & = 4(\lambda_1\lambda_4 - \lambda_2\lambda_3)^2, \\ \mathcal{C}_{AC}^2 & = 4(\lambda_2\lambda_4 - \lambda_1\lambda_3)^2, \\ \mathcal{C}_{BC}^2 & = 4(\lambda_3\lambda_4 - \lambda_1\lambda_2)^2. \end{cases} \quad (3.22)$$

From Eqs. (3.22), it is clear that there can be mixed entanglement in state (3.21) since all 2- and 3-way entanglements can be greater than zero for all $\lambda_i > 0$. An obvious difference from mixed entanglement based on state (3.18) is that in mixed entanglement based on state (3.21) GHZ entanglement and W entanglement both are related to all four basis vectors. In particular, omitting any one of the four basis vectors (note that this does not mean discarding any one of the three qubits) will make the GHZ entanglement disappear.

An important feature of the set (3.20) is the possibility for exceptional cases of mixed entanglement in state (3.21). Because for all $\lambda_i > 0$, although GHZ entanglement is always greater than zero, one or more of the three kinds of bipartite entanglement can be zero for suitable values of the coefficients so that the W entanglement is equal to zero. Therefore the mixed entanglement can disappear in these exceptional cases. The typically exceptional case of the mixed entanglement is that all three kinds of bipartite entanglement are equal to zero but only 3-way entanglement is left. Combining Eqs. (3.22) and $\sum_i \lambda_i^2 = 1$, we obtain that in this case, all four coefficients are equal to $1/2$, and state (3.21) becomes

$$|\Psi\rangle = \frac{1}{2}(|001\rangle + |010\rangle + |100\rangle + |111\rangle) \quad (3.23)$$

where the GHZ entanglement achieves its maximal value $\tau = 1$. Note that we here omit the only relevant phase $e^{i\varphi}$ since from Eqs. (3.22) it is obvious that $e^{i\varphi}$ has no relation with the entanglement of the state. If the Hadamard transformations

$$\hat{H} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad (3.24)$$

are applied to the three qubits, state (3.23) is converted to the GHZ state. Hence the state (3.23) is the GHZ state in disguise in fact but with the different forms [52]. The exceptional cases mentioned above are the singular points of the mixed entanglement based on set (3.20). Therefore here we only concentrate on set (3.20) without the singular points so that state (3.21) always possesses mixed entanglement. Without the singular points, mixed entanglement based on set (3.20) is similar to the one based on set (3.17) that τ and E_W are in the two open intervals as $\tau \in (0, 1)$ and $E_W \in (0, 4/3)$.

A common character of the compositions of sets (3.17) and (3.20) for mixed entanglement is that there is no superfluous basis vector among the four basis vectors. That is, if any one of the four basis vectors in set (3.17) or (3.20) is omitted, mixed entanglement of states based on them disappears. Thus these four basis vectors in set (3.17) or (3.20) are the minimal composition for mixed entanglement, which cannot be compressed any more.

Besides the mixed entanglement, there are other cases of true tripartite entanglement in states of four basis vectors, such as only the GHZ entanglement, only the W entanglement, and the GHZ entanglement plus one or two of the three bipartite entanglements which can be called the extended GHZ entanglement in the similar way to Ref. [32]. The differences among the GHZ, W and mixed entanglements by their squared concurrences and 3-tangles are listed in Table (3.2).

Table 3.2: Values of the three squared concurrences \mathcal{C}_{AB}^2 , \mathcal{C}_{AC}^2 and \mathcal{C}_{BC}^2 , and the 3-tangle τ for the different entanglements.

Entanglement	\mathcal{C}_{AB}^2	\mathcal{C}_{AC}^2	\mathcal{C}_{BC}^2	τ
GHZ entanglement	= 0	= 0	= 0	> 0
W entanglement	> 0	> 0	> 0	= 0
Mixed entanglement	> 0	> 0	> 0	> 0

Since the three inequivalent sets of five basis vectors (3.1) can always be decomposed into a set of type (3.17) or (3.20) plus one additional basis vector, it is clear that the possibilities for entanglement include those just discussed.

3.4 Discussion

Now consider the experiment on local conversion of the GHZ state to an approximate W state reported by Walther *et al.* in [94].

In the first step of their method, they rewrite the GHZ state in the form (3.23). Then they regard that the GHZ state (3.23) is a superposition of an unwanted term, $|111\rangle$, and a W state. That is, they consider basis vector $|111\rangle$ as an unwanted term of the W state in the form (3.23). In fact, any one of the four basis vectors in the form (3.23) can be regarded as an unwanted term of the W state. Because from Eqs. (3.22), it is obvious that if any one of the four coefficients is equal to zero, the 3-tangle τ is zero while three bipartite entanglements are greater than zero, and therefore there is only W entanglement but no GHZ entanglement. Basis vectors $|001\rangle$, $|010\rangle$ and $|100\rangle$ are very familiar basis vectors of the W state, so it is quite natural to regard basis vector $|111\rangle$ as the unwanted term.

Because one cannot exactly interconvert the GHZ state and the W state each other under any LOCC, it is impossible to decrease any one of the four coefficients in state (3.23) to be zero by LOCC. Walther *et al.* propose a special scheme in which based on positive operator valued measures (POVMs, a partial quantum measurement) and classical communication, the GHZ state can be converted to an arbitrarily good approximation of the W state. The main point of their scheme is to convert the maximal GHZ entanglement of state (3.23) to mixed entanglement of state (3.21) under LOCC. From Eqs. (3.22), it is clear that the key of the experiment is to decrease the coefficient of one of the four basis vectors, say, the coefficient λ_4 of the basis vector

$|111\rangle$. With the coefficient λ_4 going to zero, GHZ entanglement τ would be going to zero while W entanglement would be going to its maximal amount $4/3$ for the three remaining coefficients going to $1/\sqrt{3}$. But the limit $\lambda_4 = 0$ is impossible under LOCC, hence the GHZ entanglement will always remain in the final state though it can be arbitrarily small. Therefore in the final state of the experiment, there is mixed entanglement where W entanglement possesses much more proportion than GHZ entanglement, that is, there is only an approximate W state but not the exact W state locally converted from the GHZ state.

Chapter 4

Entanglement Venn Diagram and Total Tangle

In the preceding chapter, we proposed the mixed entanglement in triqubit pure states in which there is not only 3-way entanglement but also three 2-way entanglements.

Following this result, we have two questions. The first question is about the detailed relation of entanglement among three qubits. Unlike classical correlations, quantum entanglement cannot be freely shared among many objects. This is the so-called monogamy of entanglement which has been discussed in [83, 106, 107]. For example, in a pure state of three qubits A , B and C , if qubit A is maximally entangled with qubit B such as in one of the Bell states

$$|\phi\rangle_{AB} = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle), \quad (4.1)$$

i.e., the entire state $|\Psi\rangle_{ABC}$ of the qubits A , B and C can be written as the tensor product of state $|\phi\rangle_{AB}$ of qubits A and B and state $|\varphi\rangle_C$ of qubit C as

$$|\Psi\rangle_{ABC} = |\phi\rangle_{AB} \otimes |\varphi\rangle_C, \quad (4.2)$$

then qubit A (also qubit B) cannot be simultaneously entangled with qubit C . Otherwise state $|\Psi\rangle_{ABC}$ would be mixed and qubits A and B are not maximally entangled with each other. Note that the maximally entangled mixed states, which are those states that, for a given mixedness [108, 109], achieve the greatest possible entanglement, have been studied (see, e.g., [109–111]). The maximal entanglement in mixed states is not the maximal entanglement we mentioned here. The maximal entanglement we mentioned here is the absolutely maximal entanglement such as in the Bell states and in the GHZ state. It has been shown in Ref. [112] that the maximal entanglement we

mentioned here is only in the pure states. A less extreme form of this restriction is if qubit A is partly entangled with qubit B , then qubit A can have only a limited entanglement with qubit C . On the other side, entanglement among the three qubits can be 2-way entanglement and (or) 3-way entanglement. How can we understand the detailed relation of entanglement among the three qubits when considering the restriction mentioned above and the 2- and 3-way entanglements together? The second question is how to quantify the total entanglement of a triqubit pure state. There can be 2- and 3-way entanglements, simultaneously, in a state. Obviously, the concurrence and the 3-tangle are not enough to quantify the total entanglement of the state. It is necessary to introduce a new quantity for the total entanglement of a triqubit pure state.

On the other hand, complementarity [113], one of the most important principles in quantum mechanics, has been connected to entanglement in biqubit systems [33]. Quantitative complementarity relations for multiqubit systems have been discussed in [34, 35].

In this chapter, we will discuss triqubit pure states based on quantitative complementarity relations. An entanglement Venn diagram and the total tangle will be introduced for characterizing entanglement. We also generalize them for N -qubit pure states and obtain several interesting results.

This chapter is organized as follows. In section 1, we discuss the entropy Venn diagram and point out the difficulty of the diagram when discussing the detailed relation of entanglement among three qubits. In section 2, we give quantitative complementarity relations for biqubit and multiqubit pure states. In section 3, we introduce the entanglement Venn diagram and clearly classify different entanglements of triqubit pure states. In section 4, we introduce the total tangle $\tau^{(T)}$ for quantifying the total entanglement of a triqubit pure states by defining the union I that is equivalent to the total tangle $\tau^{(T)}$ from the mathematical point of view. In the final section, we generalize the entanglement Venn diagram and the union I for N -qubit pure states where we obtain bounds to the union I and a speculative formula for the union I for N -qubit pure states.

4.1 Entropy Venn diagram

Based entirely on density matrices of quantum systems, Cerf and Adami [114–116] presented a quantum mechanical extension of classical information theory, i.e., quantum information theory, that allows for a consistent description of entanglement. They found that unlike in classical information theory, quantum conditional entropies can be negative when quantum en-

tangled systems are considered. This phenomenon is completely forbidden in classical information theory. The entropy Venn diagrams of three limiting cases for the biqubit state have been drawn [115] to clearly illustrate the new phenomenon. The concept of negative conditional entropies and the entropy Venn diagram provide interesting insights into quantum entanglement.

Let us start from some simple introduction to classical information theory (see, e.g., [1]). Consider a composite system of two classical variables A and B . The Shannon entropy $H(A)$ (sometimes also called the classical entropy) of A is defined as a function of the probabilities of the different possible values $\{a\}$ that the variable A takes,

$$H(A) = - \sum_a p(a) \log_2 p(a) \quad (4.3)$$

where the variable A takes on value a with probability $p(a)$. Note that $\lim_{x \rightarrow 0} (x \log_2 x) = 0$. The Shannon entropy $H(A)$ measures the amount of uncertainty about A before we learn its value. From the viewpoint of the information theory, the Shannon entropy of A quantifies how much information we obtain, on average, when we learn the value of A . An analogous definition holds for $H(B)$. Then the joint entropy $H(A, B)$ of variables A and B is defined as

$$H(A, B) = - \sum_{a,b} p(a, b) \log_2 p(a, b), \quad (4.4)$$

which measures the total uncertainty about the pair (A, B) . The Shannon entropy of A conditional on B (Shannon conditional entropy $H(A|B)$) is therefore defined as

$$H(A|B) = H(A, B) - H(B) = - \sum_{a,b} p(a, b) \log_2 p(a|b) \quad (4.5)$$

where $p(a|b) = p(a, b)/p(b)$ is the probability of a conditional on b . $H(A|B)$ quantifies the remaining uncertainty about A when B is learned. The mutual entropy $H(A : B)$ (also denoted as $H(A \cap B)$) content of variables A and B is written as

$$H(A : B) = H(A) + H(B) - H(A, B), \quad (4.6)$$

which measures how much information the variables A and B have in common. In other words, it quantifies the (classical) correlations between the two variables A and B .

From the definitions of these entropies, we have the following equations:

$$\begin{cases} H(A : B) = H(A) - H(A|B), \\ H(A : B) = H(B) - H(B|A). \end{cases} \quad (4.7)$$

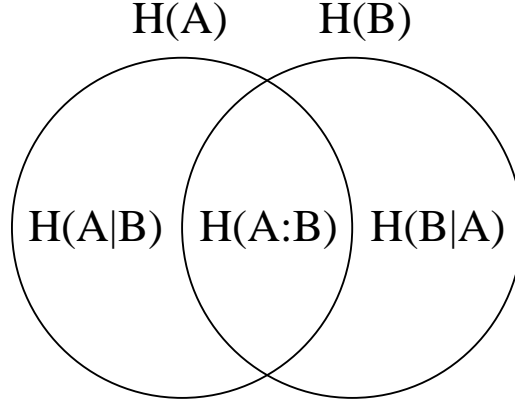


Figure 4.1: Entropy Venn diagram for the bipartite systems A and B .

All of the various relations among different entropies can be deduced from the entropy Venn diagram shown in Fig. (4.1).

In classical information theory, the conditional probability $p(x|y)$ is a number between 0 and 1, i.e., $p(x|y) \in [0, 1]$. Then the Shannon conditional entropies are always non-negative, i.e.,

$$\begin{cases} H(A|B) \geq 0, \\ H(B|A) \geq 0. \end{cases} \quad (4.8)$$

Thus the Shannon mutual entropy $H(A : B)$ cannot be greater than the entropies of any subsystem A or B , i.e.,

$$H(A : B) \leq \min\{H(A), H(B)\}. \quad (4.9)$$

Now consider a quantum system of two qubits A and B . We denote the density matrix of the entire state as ρ_{AB} and the two reduced density matrices as ρ_A and ρ_B . The von Neumann entropy $S(A)$ (sometimes also called the quantum entropy) of quantum state ρ_A is defined as

$$S(A) = -\text{Tr}(\rho_A \log_2 \rho_A). \quad (4.10)$$

Note that $\lim_{\rho \rightarrow 0}(\rho \log_2 \rho) = 0$ as for the Shannon entropy. If $\lambda_i^{(A)}$ are the eigenvalues of ρ_A , then $S(A)$ can be re-expressed as

$$S(A) = -\sum_i (\lambda_i^{(A)} \log_2 \lambda_i^{(A)}). \quad (4.11)$$

An analogous definition also holds for $S(B)$.

By analogy with the Shannon entropies, we have the following definitions of the von Neumann entropies. The von Neumann joint entropy $S(A, B)$ is defined as

$$S(A, B) = -\text{Tr}(\rho_{AB}\log_2\rho_{AB}). \quad (4.12)$$

The von Neumann conditional entropy $S(A|B)$ is defined as

$$S(A|B) = S(A, B) - S(B) = -\text{Tr}(\rho_{AB}\log_2\rho_{A|B}) \quad (4.13)$$

where $\rho_{A|B}$ is a conditional ‘‘amplitude’’ matrix as

$$\log_2\rho_{A|B} = \log_2\rho_{AB} - \log_2(\hat{I}_A \otimes \rho_B) \quad (4.14)$$

$\hat{I}_A = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ is the unit matrix in the Hilbert space \mathcal{H}_A of qubit A . Thus $S(A|B)$ can be written as

$$S(A|B) = -\text{Tr}(\rho_{AB}\log_2\rho_{AB}) + \text{Tr}(\rho_{AB}\log_2(\hat{I}_A \otimes \rho_B)). \quad (4.15)$$

The matrix $\rho_{A|B}$ is a quantum generalization of the classical conditional probability $p(a|b)$, and it can be reduced to $p(a|b)$ in the classical limit (that is, ρ_{AB} has no non-diagonal elements). The von Neumann mutual entropy $S(A : B)$ (also denoted as $S(A \cap B)$) is defined as

$$S(A : B) = S(A) + S(B) - S(A, B). \quad (4.16)$$

The Venn diagram of the von Neumann entropy, the analogy with the entropy Venn diagram in quantum case, is shown in Fig. (4.2).

Though the von Neumann entropy can be considered a generalization of the Shannon entropy, some properties of the Shannon entropy fail to hold for the von Neumann entropy. This new phenomenon has many interesting consequences for quantum information theory.

Consider the von Neumann conditional entropy $S(A|B)$. We refer to $\rho_{A|B}$ as the ‘‘amplitude’’ matrix to emphasize that it retains the quantum phases while the classical probability $p(a|b)$ has no such content. However $\rho_{A|B}$ is not a density matrix but a Hermitian and positive semi-definite matrix (so its eigenvalues are real and non-negative), since its eigenvalues can exceed 1. That is, in the classical case, $p(a|b)$, as a probability distribution in a conditional on b , satisfies $0 \leq p(a|b) \leq 1$; but its quantum analogy $\rho_{A|B}$ does NOT satisfy $0 \leq \rho_{A|B} \leq 1$ since it can have an eigenvalue greater than 1. Here the notation $\rho_{A|B} \leq 1$ means that the matrix $(\hat{I}_A - \rho_{A|B})$ is positive semi-definite. The consequence is that the von Neumann conditional entropy can be negative, a new important phenomenon in quantum information theory.

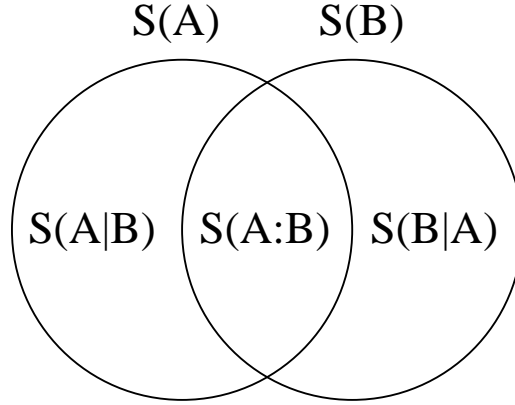


Figure 4.2: Venn diagram of the von Neumann entropies for quantum system of qubits A and B .

For example, let a quantum system of two qubits A and B be in one of the Bell states

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle). \quad (4.17)$$

Two reduced density matrices ρ_A and ρ_B are

$$\rho_A = \rho_B = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (4.18)$$

Then two von Neumann conditional entropies $S(A|B)$ and $S(B|A)$ are

$$\begin{cases} S(A|B) = S(A, B) - S(B) = -1, \\ S(B|A) = S(A, B) - S(A) = -1. \end{cases} \quad (4.19)$$

Thus the negativity of the conditional von Neumann entropies necessarily results from $\rho_{A|B}$ admitting an eigenvalue greater than 1. From Eqs. (4.19), $S(A|B) < 0$ means the entropy of the entire system AB , $S(A, B)$, can be less than the entropy of one of its subsystems, a situation which is of course forbidden in classical information theory.

From the subadditivity inequality for von Neumann entropies

$$S(A, B) \leq S(A) + S(B) \quad (4.20)$$

with equality if and only if $\rho_{AB} = \rho_A \otimes \rho_B$, we obtain

$$S(A|B) \leq S(A). \quad (4.21)$$

From the triangle (sometimes also called Araki-Lieb) inequality

$$S(A, B) \geq |S(A) - S(B)|, \quad (4.22)$$

we obtain

$$S(A|B) \geq -S(A). \quad (4.23)$$

Thus

$$|S(A|B)| \leq S(A), \quad (4.24)$$

which is different from the first inequality in Ineqs (4.8). These properties also hold for $S(B|A)$.

Let us consider the relation between the negativity of the conditional von Neumann entropy and entanglement. If ρ_{AB} is separable, i.e.,

$$\rho_{AB} = \sum_i p_i \rho_A^i \otimes \rho_B^i \quad (4.25)$$

where $p_i > 0$ are the probabilities of pure states $\rho_{AB}^i = \rho_A^i \otimes \rho_B^i$, then

$$(\hat{I}_A \otimes \rho_B) - \rho_{AB} = \sum_i p_i (\hat{I}_A - \rho_A^i) \otimes \rho_B^i. \quad (4.26)$$

Since ρ_A^i and ρ_B^i are density matrices, $(\hat{I}_A - \rho_A^i) \geq 0$ and $\rho_B^i \geq 0$ always hold. Thus, as the sum of positive matrices,

$$(\hat{I}_A \otimes \rho_B) - \rho_{AB} \geq 0 \quad (4.27)$$

always holds. Therefore the matrix $(-\log_2 \rho_{A|B})$ is positive semi-definite. This immediately implies that

$$\rho_{A|B} \leq 1 \quad (4.28)$$

always holds for the separable state. Consequently, a necessary condition for separability of state ρ_{AB} is that all the eigenvalues of the conditional amplitude matrices $\rho_{A|B}$ and $\rho_{B|A}$ are NOT greater than 1, i.e., the conditional von Neumann entropies $S(A|B)$ and $S(B|A)$ are not negative. Therefore the negativity of the conditional von Neumann entropy straightway implies entanglement of quantum systems.

For the von Neumann mutual entropy $S(A : B)$, combining Eqs. (4.16) and (4.19), we obtain

$$S(A : B) = S(A) - S(A|B). \quad (4.29)$$

Eq. (4.29) obviously shows that $S(A : B)$ can be greater than the entropy of subsystem A since $S(A|B)$ can be negative, while its classical analogy

$H(A : B)$ cannot be greater than the entropy of any of the subsystems. Using Ineqs. (4.20) and (4.22), we obtain

$$0 \leq S(A : B) \leq 2\min\{S(A), S(B)\}, \quad (4.30)$$

which is different from Ineq. (4.9).

As the generalization of the Shannon mutual entropy $H(A : B)$, the von Neumann mutual entropy $S(A : B)$ measures not only quantum correlations (i.e., entanglement) but also classical correlations between two qubits A and B . In the classical limit, $S(A : B)$ reduces to $H(A : B)$. But the von Neumann mutual entropy can NOT discriminate purely quantum correlations (entanglement) from classical correlations. There are three limiting cases of the correlations between two qubits A and B : completely independent, the maximal classical correlation and the maximal entanglement. Their entropy Venn diagrams are shown in Fig. (4.3).

In Fig. (4.3-I), two qubits are completely independent. The state of the entire system is the tensor product of the states of two qubits A and B , and each qubit is in the maximally mixed state, i.e.,

$$\begin{aligned} \rho_A = \rho_B &= \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \\ \rho_{AB} = \rho_A \otimes \rho_B &= \frac{1}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \end{aligned} \quad (4.31)$$

Thus

$$\begin{cases} \rho_{A|B} = \rho_A \otimes \hat{I}_B \Rightarrow S(A|B) = S(A) = 1 \\ \rho_{B|A} = \hat{I}_A \otimes \rho_B \Rightarrow S(B|A) = S(B) = 1 \end{cases} \implies S(A : B) = 0. \quad (4.32)$$

In Fig (4.3-II), two qubits have the maximal classical correlations but no entanglement. The entire state is the 50/50 mixture of states $|00\rangle\langle 00|$ and $|11\rangle\langle 11|$ or states $|01\rangle\langle 01|$ and $|10\rangle\langle 10|$, for example,

$$\begin{aligned} \rho_A = \rho_B &= \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \\ \rho_{AB} &= \frac{1}{2}(|00\rangle\langle 00| + |11\rangle\langle 11|) = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \end{aligned} \quad (4.33)$$

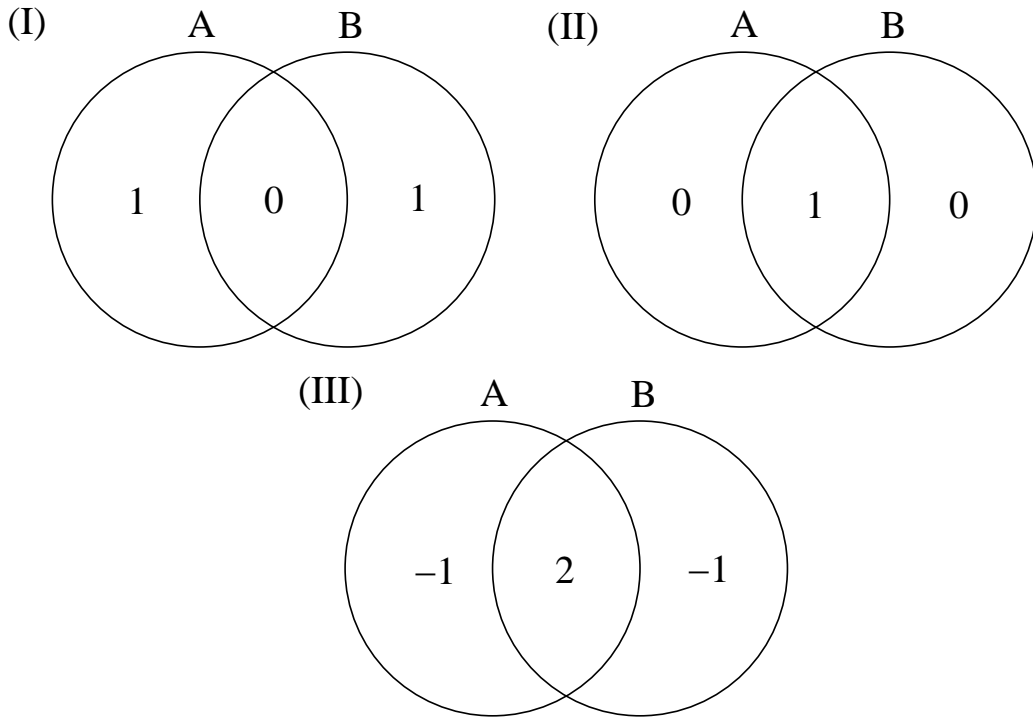


Figure 4.3: Entropy Venn diagrams of biqubit states AB for three limiting cases. Here we select $S(A) = S(B) = 1$. (I): Two qubits A and B are completely independent, i.e., without classical and quantum correlations. (II): Two qubits have the maximal classical correlations but no entanglement. (III): Two qubits are maximally entangled, where $S(A|B)$ and $S(B|A)$ both get their minimal value -1 , and $S(A : B)$ gets the maximal value 2 , which are completely forbidden in the classical cases.

Thus

$$\begin{cases} S(A|B) = S(B|A) = 0, \\ S(A : B) = 1. \end{cases} \quad (4.34)$$

All properties of systems in Figs. (4.3-I) and (4.3-II) correspond with the properties of the Shannon entropies.

In Fig. (4.3-III), two qubits are maximally entangled with each other. The entire state is one of the Bell states while the two reduced states are the

maximally mixed states, for example,

$$\rho_{AB} = \frac{1}{2}(|00\rangle + |11\rangle)(\langle 00| + \langle 11|) = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}. \quad (4.35)$$

$$\rho_A = \rho_B = \frac{1}{2}(|0\rangle\langle 0| + |1\rangle\langle 1|) = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

Thus

$$\begin{cases} S(A|B) = S(B|A) = -1, \\ S(A : B) = 2. \end{cases} \quad (4.36)$$

This case is forbidden in classical information theory.

It has been pointed out that the negativity of conditional entropies result from entanglement. The entropy Venn diagrams for biqubit states clearly illustrate the difference between classical correlations and quantum correlations, i.e., entanglement. Since entropy Venn diagrams of biqubit states can help us understand entanglement between two qubits, we naturally have the idea to generalize the entropy Venn diagram for more than two qubits.

Let us consider the generalization of the entropy Venn diagram for triqubit pure states, the simplest instance of multipartite quantum systems. The various concepts of the von Neumann entropy for biqubit states can be generalized to the ones for triqubit states as follows. The entropy Venn diagram for a triqubit state is shown in Fig. (4.4).

The basic concepts of the von Neumann entropy for triqubit states can be straightforwardly generalized from the ones of biqubit states, such as $S(A)$, $S(B)$, $S(C)$, the bi-joint entropies $S(A, B)$, $S(A, C)$ and $S(B, C)$, and the tri-joint entropy $S(A, B, C)$. Conditional entropies, such as $S(A|(B, C))$, $S(B|(A, C))$ and $S(C|(A, B))$, quantify the entropy of one of the three subsystems when the other two subsystems are known. For example, $S(A|(B, C))$ is written in analogy with Eq. (4.13) as

$$S(A|(B, C)) = S(A, B, C) - S(B, C). \quad (4.37)$$

Conditional entropies, such as $S((A, B)|C)$, $S((A, C)|B)$ and $S((B, C)|A)$, quantify the entire entropy of two of the three subsystems when the last subsystem is known. For example, $S((A, B)|C)$ is written as

$$S((A, B)|C) = S(A, B, C) - S(C). \quad (4.38)$$

Mutual conditional entropies, such as $S((A : B)|C)$, $S((A : C)|B)$ and $S((B : C)|A)$, quantify the bi-mutual entropy between two of the three subsystems

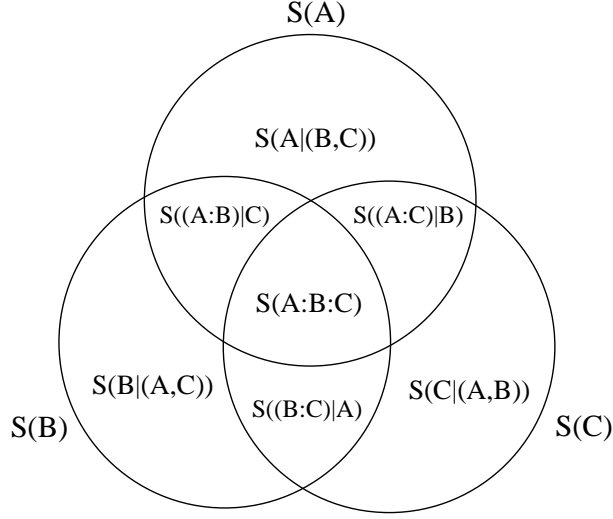


Figure 4.4: Entropy Venn diagram for a state of three qubits A , B and C .

when the last subsystem is known. For example, $S((A : B)|C)$ is written in analogy to Eq. (4.29) as

$$\begin{aligned} S((A : B)|C) &= S(A|C) - S(A|(B, C)) \\ &= S(A, C) + S(B, C) - S(C) - S(A, B, C). \end{aligned} \quad (4.39)$$

The tri-mutual entropy $S(A : B : C)$ (also denoted as $S(A \cap B \cap C)$) is written in analogy to Eq. (4.29) as

$$S(A : B : C) = S(A : B) - S((A : B)|C). \quad (4.40)$$

Using Eq. (4.39), $S(A : B : C)$ can be written in detail as

$$\begin{aligned} S(A : B : C) &= S(A) + S(B) + S(C) \\ &\quad - S(A, B) - S(A, C) - S(B, C) + S(A, B, C). \end{aligned} \quad (4.41)$$

In the preceding section, we have pointed out that there are the GHZ entanglement, the W entanglement and the mixed entanglement as the form of the true tripartite entanglement in triqubit pure states. We draw entropy Venn diagrams for the GHZ state and the W state in Fig. (4.5). From Fig. (4.5), we found that it is not enough to exactly detect the class of entanglement of a triqubit pure state according to its entropy Venn diagram. Only for the GHZ state, the diagram is sufficient. But for the W state, the state with the non-maximal GHZ entanglement and the state with the mixed entanglement, entropy Venn diagrams are not enough to distinguish them.

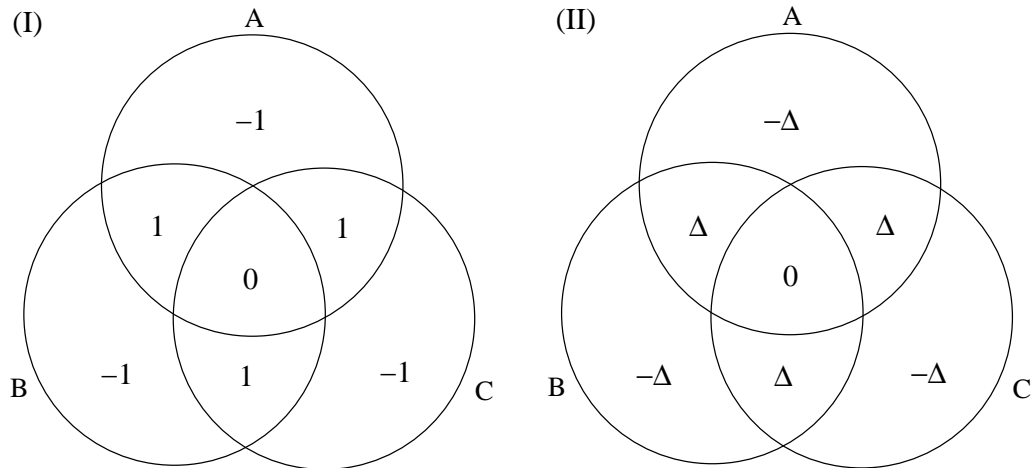


Figure 4.5: Entropy Venn diagrams for the GHZ state (I) and the W state (II), where $\Delta = \log_2 3 - 2/3 \approx 0.9183$.

That is, in general, entropy Venn diagrams can NOT show us the detailed situation of entanglement in triqubit pure states. There is no difference between 2- and 3-way entanglements in entropy Venn diagrams.

Thus from the viewpoint of understanding detailed entanglement among three qubits and characterizing (including classifying and quantifying) entanglement of triqubit pure states, the entropy Venn diagram is not a good tool though it is well known that the concept of entropy is the most important parameter in the information theory.

4.2 Quantitative complementarity relations

Complementarity, first introduced by Niels Bohr in 1928 [113], is one of the most important principles in quantum mechanics. The concept of complementarity (see, e.g., [117, 118]) in its full generality states that a quantum system may possess properties that are equally real but mutually exclusive. It is well known that in classical world, the objects can be precisely described with the completeness demanded by classical dynamics. For example, we can unambiguously combine the space-time coordinates of objects with the dynamical conservation laws that govern their mutual interactions. However, in quantum world, the precise description of a quantum object, in general, is precluded by complementarity. Some of the elements that complement each other to make up a complete classical description of a quantum object are actually mutually exclusive, and these complementary elements are all

necessary for the description of various aspects of the quantum object.

An alternative statement of complementarity, which makes reference to experimental arrangements or measurements, states that information about a quantum object obtained under different experimental arrangements cannot always be comprehended within a single causal picture. Thus, from the experimental point of view, complementarity in quantum world can be considered as the natural generalization of the classical concept of causality though they are quite different in nature.

This is not to be regarded as a deficiency of the experimenter or the experimental techniques. It is rather a law of nature that, whenever an attempt is made to measure precisely one of the pair of canonical variables, the other is changed by an amount that cannot be too closely calculated without interfering with the primary attempt. This is fundamentally different from the classical situation, in which a measurement also disturbs the system that is under observation, but the amount of the disturbance can be calculated and taken into account. Thus, Bohr has pointed out that complementarity implies the “impossibility of any sharp separation between the behavior of atomic (quantum) objects and their interaction with the measuring instruments which serve to define the conditions under which the phenomena appear” [113]. Therefore the complementarity principle typifies the fundamental limitations on the classical concept that the behavior of quantum systems can be described independently of the means by which they are observed.

In single quantum systems, there are two typical examples of complementarity. The first example is the uncertainty principle, developed by Heisenberg in 1927 [119]. According to this principle, it is impossible to specify precisely and simultaneously the values of both members of particular pairs of physical variables that describe the behavior of a quantum system. The members of these pairs of variables are canonically conjugate to each other in the hamiltonian sense, for example, the rectangular coordinate x of a particle and the corresponding component of momentum p_x . To put it more quantitatively, the uncertainty principle states that the order of magnitude of the product of the uncertainties in the knowledge of the two variables must be at least \hbar (Planck’s constant h divided by 2π) as

$$\Delta x \cdot \Delta p_x \gtrsim \hbar. \quad (4.42)$$

This relation means that a component of the momentum of a particle cannot be precisely specified without loss of all knowledge of the corresponding component of its position at that time, that a particle cannot be precisely localized in a particular direction without loss of all knowledge of its momentum component in that direction, and that in intermediate cases the product

of the uncertainties of the simultaneously measurable values of corresponding position and momentum components is at least of the order of magnitude of \hbar . The smallness of Planck's constant h makes the uncertainty principle of interest primarily in connection with systems of quantum size.

The second example of complementarity in single quantum systems is the wave-particle duality of a photon, a long-standing debate over the nature of light [120]. This type of complementarity is often illustrated by means of two-way interferometers: A classical particle can take only one path, while a classical wave can pass through both paths and therefore display interference fringes when the two partial waves are recombined. Depending on their state, quantum mechanical systems, such as photons, electrons, and so on, can behave like particles (go along a single path), like waves (show interference), or remain in between these extreme cases by exhibiting particlelike as well as wavelike behavior (this is the so-called wave-particle duality).

Two quantities have been introduced for the wave-particle duality of quantons: the visibility V of the interference fringes after recombination of the two partial waves, which quantifies the wavelike behavior, and the predictability P , which measures the probability that the system will go along a specific path, i.e., the particlelike behavior. A quantitative expression for the complementarity [121–126] is the inequality

$$V^2 + P^2 \leq 1, \quad (4.43)$$

which states that the more particlelike a system behaves, the less pronounced the wavelike behavior becomes.

In composite quantum systems consisting of two or more quantum particles, complementarity has been studied in the last few years. Some important progress has been made, such as complementarity relations between single and two-particle fringe visibilities [123,124], between distinguishability and visibility [125], between the coherence and predictability in a quantum eraser [126], and so on, and some of them have been experimentally verified (see, e.g., [127]).

On another hand, the concept of entanglement is involved inevitably in the study of composite quantum systems. Naturally, we would like to ask whether entanglement that constitutes a physical feature of quantum systems can be incorporated into complementarity. Some authors have explored this question and obtained some important results, such as complementarity relations between coherence and entanglement [128], between distinguishability and entanglement [129], between local and nonlocal information [130], between multipartite entanglement and mixedness for special classes of N -qubit systems [131], and so on.

Recently, Jakob and Bergou [33] made an important progress by deriving quantitative complementarity relations for qubit pure states. They showed that an arbitrary normalized pure state $|\Psi\rangle_{AB}$ of qubits A and B satisfies the expression

$$\mathcal{C}^2 + S_k^2 = 1 \quad (4.44)$$

for $k \in \{A, B\}$. Here \mathcal{C} denotes the concurrence between qubits A and B , i.e., quantifies the entanglement between qubits A and B . S_k^2 denotes the single entity of the single partite properties (wave-particle duality) of qubit k and is written as

$$S_k^2 = V_k^2 + P_k^2. \quad (4.45)$$

Additionally, Jakob and Bergou have noted that Eq. (4.44) becomes an inequality when applied to a qubit mixed state.

In the language of quantum information theory, the quantitative complementarity relations (4.44) can be understood in such a way that the reality of qubit k in a qubit pure state is separated into two parts: the nonlocal reality (i.e., entanglement) and the local reality (i.e., the single particle properties). Here the quantity \mathcal{C}^2 measures the nonlocal reality of qubit k and the quantity S_k^2 measures its local reality. It has been shown that the concurrence \mathcal{C} remains invariant under local unitary transformations [80]. For the single entity S_k^2 of qubit k , though its two constituents V_k^2 and P_k^2 can be changed under local unitary transformations into $(V'_k)^2$ and $(P'_k)^2$, they satisfy the condition

$$V_k^2 + P_k^2 = (V'_k)^2 + (P'_k)^2, \quad (4.46)$$

so that the entity S_k^2 remains unchanged. In particular, S_k^2 can be all visibility with no predictability or, alternatively, all predictability with no visibility.

All quantities in Eqs. (4.44) and (4.45) can be calculated from the density matrix of the initial state and the reduced density matrices. The detailed method of calculating the concurrence \mathcal{C} has been displayed in the preceding chapter. Here we only consider the visibility V_k and the predictability P_k of qubit k . First, let us introduce the single-qubit reduced density matrix ρ_k , which is defined as

$$\rho_k \equiv \text{Tr}_j(\rho) \quad (4.47)$$

for $j \neq k$. Here ρ is the density matrix of the initial qubit pure state. The visibility V_k , which quantifies, e.g., the fringe visibility in the context of two-slit interference experiments, is written as

$$V_k = 2|\text{Tr}(\rho_k \sigma_+^{(k)})| \quad (4.48)$$

where

$$\sigma_+^{(k)} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad (4.49)$$

is the raising operator acting on qubit k . The predictability P_k , which quantifies, e.g., the *a priori* information whether the particle is more likely to take the upper or lower path in an interferometer, is written as

$$P_k = |\text{Tr}(\rho_k \sigma_z^{(k)})| \quad (4.50)$$

where

$$\sigma_z^{(k)} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (4.51)$$

is one of Pauli matrices acting on qubit k .

More recently, Tessier in [34] and Peng *et al.* in [35] generalized quantitative complementarity relations to multiqubit pure systems. Especially, Peng *et al.* in [35] have experimentally verified some of quantitative complementarity relations in a biqubit system using nuclear magnetic resonance techniques.

For a pure state of N qubits A_1, A_2, \dots, A_N , the following quantitative complementarity relations were suggested [34, 35]

$$\tau_{k(R_k)} + S_k^2 = 1 \quad (4.52)$$

where $k = 1, 2, \dots, N$ and R_k denotes the set of the $(N-1)$ qubits other than qubit A_k . Similarly to the case of biqubit pure states, $\tau_{k(R_k)}$ quantifies the nonlocal reality of qubit A_k , which measures entanglement between qubits A_k and the remaining $(N-1)$ qubits and remains invariant under local unitary transformations. S_k^2 quantifies the local reality, i.e., the single particle property, of qubit A_k as shown in the case of biqubit pure states. $\tau_{k(R_k)}$, the squared I -concurrence proposed in [81] indeed, is given by

$$\tau_{k(R_k)} = 2[1 - \text{Tr}(\rho_k^2)]. \quad (4.53)$$

Here the single-qubit reduced density matrix ρ_k of N -qubit state is given by

$$\rho_k \equiv \text{Tr}_{\{j\}}(\rho) \quad (4.54)$$

for $\{j | \text{all } j \neq k\}$ where ρ is the density matrix of the initial N -qubit pure state.

By Eq. (4.80), $\tau_{k(R_k)}$ and S_k^2 satisfy the following inequalities

$$\begin{cases} 0 \leq \tau_{k(R_k)} \leq 1, \\ 0 \leq S_k^2 \leq 1. \end{cases} \quad (4.55)$$

The two extremal cases for qubit A_k are $\tau_{k(R_k)} = 1$ ($S_k^2 = 0$), for example, in the N -qubit GHZ state [92], and $\tau_{k(R_k)} = 0$ ($S_k^2 = 1$), for example, in a fully separable state.

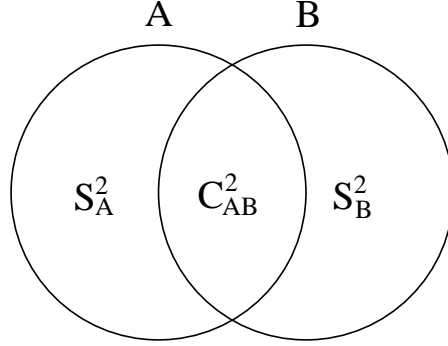


Figure 4.6: Entanglement Venn diagram for state ρ of two qubits A and B . The common area of two qubits, denoted as \mathcal{C}_{AB}^2 , means entanglement between the two qubits A and B . The two remaining areas of qubits A and B , denoted as S_A^2 and S_B^2 , mean the single-partite properties of the two qubits A and B , respectively.

4.3 Entanglement Venn diagram

It has been shown that the entropy Venn diagram provides some interesting insights into quantum entanglement in biqubit states. However, it meets some difficulty to show the detailed entanglement in multiqubit systems. In this section, we introduce entanglement Venn diagrams for biqubit and triqubit pure states based on quantitative complementarity relations. With them, we can clearly understand the detailed entanglement among the qubits, especially in triqubit pure states in which the entropy Venn diagram meets some difficulty. This allows us to further discuss entanglement of multiqubit systems. First, we will introduce entanglement Venn diagrams for biqubit pure states and compare them to entropy Venn diagrams. Then we will introduce entanglement Venn diagrams for triqubit pure states and discuss the classification of triqubit entanglement by different forms of entanglement Venn diagrams.

First consider a pure state ρ of two qubits A and B . Quantitative complementarity relations can be written as

$$\begin{cases} \mathcal{C}_{AB}^2 + S_A^2 = 1, \\ \mathcal{C}_{AB}^2 + S_B^2 = 1. \end{cases} \quad (4.56)$$

That is, each qubit is composed of two parts: the nonlocal reality quantified by \mathcal{C}^2 and the local reality S^2 . The entanglement Venn diagram of state ρ is shown in Fig. (4.6).

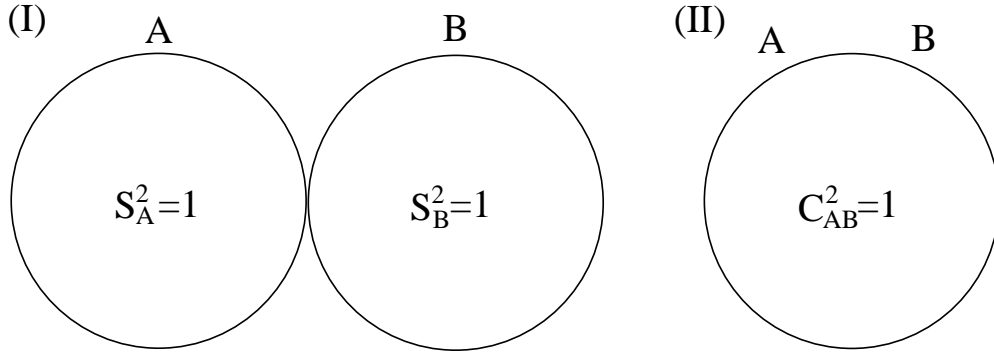


Figure 4.7: Entanglement Venn diagrams of biqubit pure states for two extremal cases of entanglement: (I) for separable states as two disjoint circles; (II) for the maximally entangled states as one circle, which means the entire overlap of the two qubits.

In Fig. (4.6), each qubit is represented by a circle with two parts corresponding to the two realities of the qubit. The common area of the two qubits means their entanglement and is quantified by the squared concurrence \mathcal{C}_{AB}^2 . The relative complement of qubit B in qubit A , $A|B$, expresses the single-partite property S_A^2 of qubit A . Similarly, the relative complement of qubit A in qubit B , $B|A$, expresses the single-partite property S_B^2 of qubit B .

In contrast to the correlations (including classical and quantum correlations) between the two qubits in state ρ , there are only two cases between the two qubits, separable or entangled, from the entanglement point of view. The two extremal cases of entanglement between the two qubits A and B , separable ($\mathcal{C}_{AB}^2 = 0$) and maximally entangled ($\mathcal{C}_{AB}^2 = 1$), are shown in Fig. (4.7).

For separable states, there is no entanglement between the two qubits, i.e., $\mathcal{C}_{AB}^2 = 0$, while the single-partite properties S_A^2 and S_B^2 both are the maximum 1. Thus there are two disjoint circles in the entanglement Venn diagram as Fig. (4.7-I). For entangled states, there is certainly a common area between the two qubits in entanglement Venn diagrams. If the entanglement \mathcal{C}_{AB}^2 of the states achieves its maximum 1, then S_A^2 and S_B^2 both are the minimum 0. The corresponding entanglement Venn diagram is shown as one circle in Fig. (4.7-II).

Now consider a pure state of three qubits A , B and C . Quantitative complementarity relations can be written as

$$\tau_{i(jk)} + S_i^2 = 1 \quad (4.57)$$

where $i, j, k \in \{A, B, C\}$. The nonlocal reality $\tau_{i(jk)}$ of qubit i , i.e., entanglement between qubit i and pair of qubits (jk) , can be presented as [83]

$$\tau_{i(jk)} = \tau + \mathcal{C}_{ij}^2 + \mathcal{C}_{ik}^2 \quad (4.58)$$

where τ is the 3-tangle quantifying 3-way entanglement among all three qubits together, \mathcal{C}_{ij}^2 (or \mathcal{C}_{ik}^2) is the squared concurrence quantifying 2-way entanglement between qubits i and j (or k). Then we obtain three detailed quantitative complementarity relations as

$$\begin{cases} \tau + \mathcal{C}_{AB}^2 + \mathcal{C}_{AC}^2 + S_A^2 = 1, \\ \tau + \mathcal{C}_{AB}^2 + \mathcal{C}_{BC}^2 + S_B^2 = 1, \\ \tau + \mathcal{C}_{AC}^2 + \mathcal{C}_{BC}^2 + S_C^2 = 1, \end{cases} \quad (4.59)$$

where $0 \leq \tau, \mathcal{C}^2_s, S^2_s \leq 1$.

From these relations, we can see a two-step separation of a qubit, for example, qubit A , in triqubit pure states. In the first step, we separate qubit A into two parts, the nonlocal reality $\tau_{A(BC)}$ and the local reality S_A^2 , as Eq. (4.57). In the second step, we sequentially separate the nonlocal reality $\tau_{A(BC)}$ into two kinds of parts, one kind related with 3-way entanglement τ and another kind with two 2-way entanglements \mathcal{C}_{AB}^2 and \mathcal{C}_{AC}^2 . In the end, qubit A is separated into three different kinds of parts, one related with the single-partite property S_A^2 , one with the two 2-way entanglements \mathcal{C}_{AB}^2 and \mathcal{C}_{AC}^2 , and one with the 3-way entanglement τ .

Representing each of the three qubits as a circle, we draw an entanglement Venn diagram for a triqubit pure state in Fig. (4.8) to intuitively illustrate entanglement among the three qubits. With the mathematical terminology of set theory, we explain the physical meanings of every subarea in Fig. (4.8). Consider qubit A as the focus, shown as a bold-faced circle in Fig. (4.8). The relative complement of pair of qubits (BC) in qubit A , $A|(B \cup C)$, expresses the single particle property S_A^2 of qubit A . The intersection of qubit A with pair of qubits (BC) , $A \cap (B \cup C)$, expresses entanglement $\tau_{A(BC)}$ between qubit A and pair of qubits (BC) . The intersections $(A \cap B)|C$ and $(A \cap C)|B$ express 2-way entanglements \mathcal{C}_{AB}^2 and \mathcal{C}_{AC}^2 of qubit A with B and with C , respectively. The intersection $A \cap B \cap C$ expresses 3-way entanglement τ among all three qubits together. The cases of qubits B and C are similar to the one of qubit A .

Now consider the different types of entanglement in triqubit pure states. The first type is fully separable states denoted as $\rho \in \{1^3\} = \{\text{states with form } \rho_A \otimes \rho_B \otimes \rho_C\}$. There is no common area among the three qubits in the entanglement Venn diagram as shown in Fig. (4.9-I). The second type is biseparable states denoted as $\rho \in \{1^1, 2^1\} = \{\text{states with form } \rho_A \otimes \rho_{BC}$,

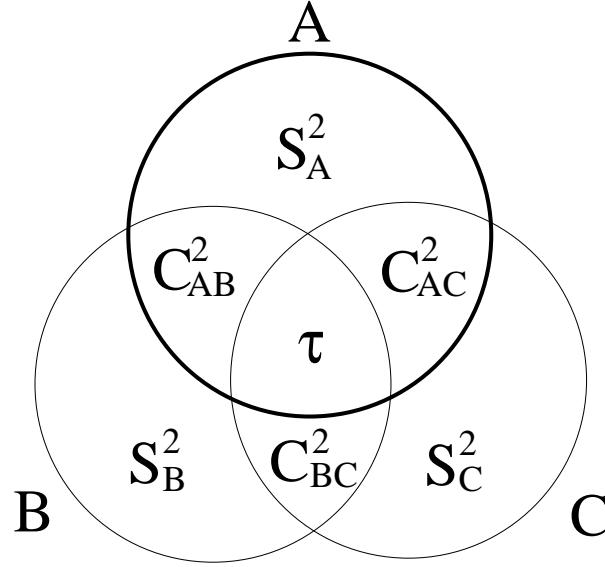


Figure 4.8: Entanglement Venn diagram for a pure state of three qubits A , B and C .

$\rho_B \otimes \rho_{AC}, \rho_C \otimes \rho_{AB}$. In these states, there is only one 2-way entanglement between two of the three qubits. That is, one of the three qubits is separable from the two remaining qubits while the two remaining qubits are entangled with each other. For example, state $\rho = \rho_A \otimes \rho_{BC}$, qubit A is separable from pair of qubits B and C while qubits B and C are entangled with each other. Quantitative complementarity relations can be written as

$$\begin{cases} S_A^2 = 1, \\ C_{BC}^2 + S_B^2 = 1, \\ C_{BC}^2 + S_C^2 = 1. \end{cases} \quad (4.60)$$

The corresponding entanglement Venn diagram is shown in Fig. (4.9-II-a) where there is no intersection between qubit A and pair of qubits BC but an intersection between qubits B and C . In the extremal case entanglement C_{BC}^2 achieves the maximum 1. Its entanglement Venn diagram is shown in Fig. (4.9-II-b) as two disjoint circles where one of the circles expresses separable qubit A and another of the circles expresses the maximal entanglement between qubits B and C .

The last type is fully entangled states denoted as $\rho \in \{3^1\} = \{\text{states with form } \rho_{ABC}\}$, including the W entanglement, the GHZ entanglement and the mixed entanglement. This entanglement is called the full entanglement of the three qubits, full entanglement for short, or the true tripartite entanglement.

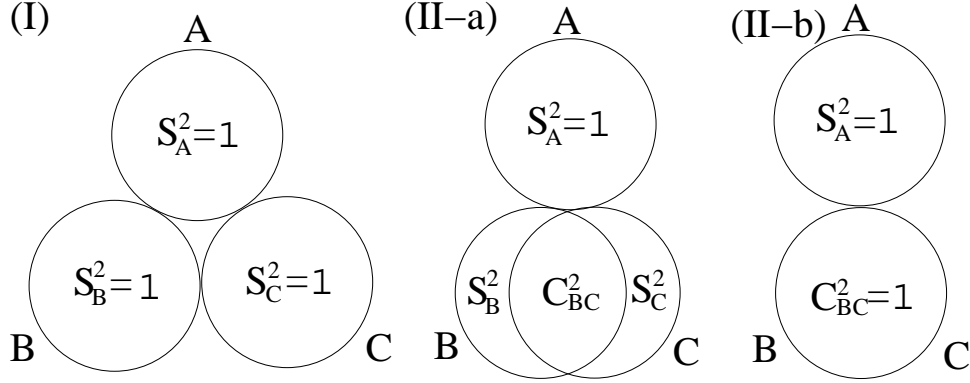


Figure 4.9: Entanglement Venn diagrams for separable and biseparable triqubit pure states: (I) for fully separable states as three disjoint circles; (II-a) for biseparable states, for example, $\rho = \rho_A \otimes \rho_{BC}$, as one disjoint circle and two joint circles; (II-b) for biseparable states with one maximal 2-way entanglement as two disjoint circles in which one circle means separable qubit A while another circle means the entire overlap of two maximally entangled qubits B and C .

For states of the W entanglement, there is no 3-way entanglement ($\tau = 0$) but three 2-way entanglements so that quantitative complementarity relations can be written as

$$\begin{cases} \mathcal{C}_{AB}^2 + \mathcal{C}_{AC}^2 + S_A^2 = 1, \\ \mathcal{C}_{AB}^2 + \mathcal{C}_{BC}^2 + S_B^2 = 1, \\ \mathcal{C}_{AC}^2 + \mathcal{C}_{BC}^2 + S_C^2 = 1. \end{cases} \quad (4.61)$$

The corresponding entanglement Venn diagram is shown in Fig. (4.10-I) as three bi-mutual joint circles without intersection of all three qubits. For states of the GHZ entanglement, there is no 2-way entanglement (\mathcal{C}^2 s = 0) but only 3-way entanglement so that there is only an intersection among the three qubits in the entanglement Venn diagram. For the GHZ state, its 3-way entanglement τ achieves its maximum 1 so that all qubits have only nonlocal realities but no local realities. Its entanglement Venn diagram is shown in Fig. (4.10-II) as one circle, the entire overlap of the three qubits. For states of mixed entanglement, all 2- and 3-way entanglements are greater than zero so that all intersections among the qubits exist in entanglement Venn diagram as Fig. (4.10-III).

With the help of these entanglement Venn diagrams, we can clearly understand the detailed entanglement among the three qubits. For different entanglements, the corresponding entanglement Venn diagrams are different. From entanglement Venn diagrams, we can also find some properties of

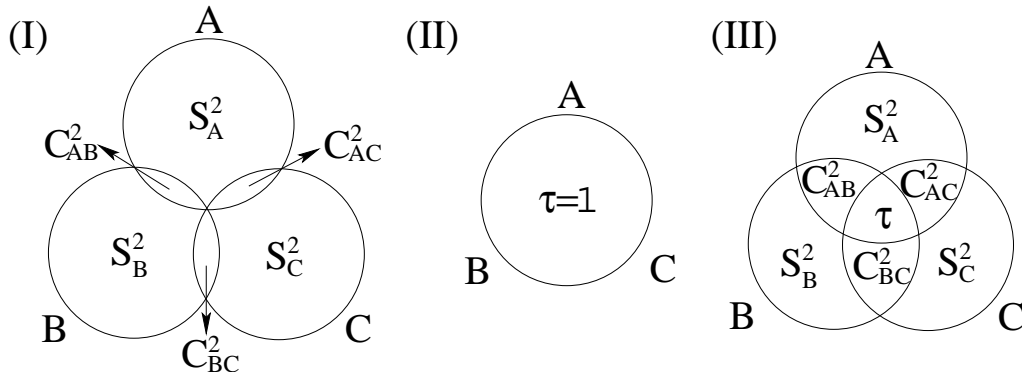


Figure 4.10: Entanglement Venn diagrams for triqubit pure states with different classes of full entanglement: (I) for the W state where there is no intersection among all three qubits together but three mutual intersections of two of the three qubits; (II) for the GHZ state as one circle, which means the entire overlap of the three qubits; (III) for states of mixed entanglement where all intersections among the qubits exist.

corresponding entanglement. In one word, we construct a one-to-one mapping between the forms of entanglement Venn diagrams and the classes of entanglement.

4.4 Total tangle

In the preceding section, we introduced entanglement Venn diagrams for triqubit pure states, in which we can clearly classify different entanglements. In this section, we will define a new quantity, named the union I , for triqubit pure states based on the entanglement Venn diagram as in Fig. (4.8). Some requirements for a quantity to be a good measure of entanglement have been listed in Chapter 2. The union I does not satisfy the normalization of the entanglement measure, one of the requirements for the entanglement measure. Thus a new quantity, named the total tangle $\tau^{(T)}$, will be introduced for quantifying the total entanglement of triqubit pure states, especially for states with mixed entanglement, by the union I . In fact, the union I and the total tangle $\tau^{(T)}$ are equivalent to each other from the mathematical point of view. This will be clear from the definition of the total tangle $\tau^{(T)}$. But being the measure of entanglement, the total tangle $\tau^{(T)}$ has some other merits than the union I according to the requirements.

It has been pointed out that there are the 2- and 3-way entanglements,

simultaneously, in states with mixed entanglement so that the squared concurrence and the 3-tangle are not enough to quantify this entanglement. For example, for two states ρ^I and ρ^{II} both with the mixed entanglement, if the W entanglement of state ρ^I is greater than the one of state ρ^{II} while the GHZ entanglement of state ρ^I is less than the one of state ρ^{II} , how can we compare total entanglement of these two states? The simplest case of such comparison is whether we can compare entanglements of two states, one with GHZ entanglement and another with W entanglement, and how to compare. These problems can be easily solved by the union I (and the total tangle $\tau^{(T)}$) which will be introduced in this section.

Based on the entanglement Venn diagram as shown in Fig. (4.8), we define the union, denoted as I , of a triqubit pure state, invoking an analogy to set theory, as

$$I = \tau + \mathcal{C}_{AB}^2 + \mathcal{C}_{AC}^2 + \mathcal{C}_{BC}^2 + S_A^2 + S_B^2 + S_C^2. \quad (4.62)$$

With Eqs. (4.59), we can rewrite Eq. (4.62) in two different ways. In the first way, by one of Eqs. (4.59), the union I can be rewritten as

$$I = 1 + \mathcal{C}_{ij}^2 + S_i^2 + S_j^2 \quad (4.63)$$

where $i, j \in \{A, B, C\}$. Since \mathcal{C}^2 s, S^2 s are greater than or equal to zero, the union I can assume the minimum value 1 when $\mathcal{C}_{ij}^2 = S_i^2 = S_j^2 = 0$ holds, for example, in the GHZ state.

In the second way, we can transform Eqs. (4.59) into the form

$$\begin{cases} S_A^2 = 1 - \tau - \mathcal{C}_{AB}^2 - \mathcal{C}_{AC}^2, \\ S_B^2 = 1 - \tau - \mathcal{C}_{AB}^2 - \mathcal{C}_{BC}^2, \\ S_C^2 = 1 - \tau - \mathcal{C}_{AC}^2 - \mathcal{C}_{BC}^2. \end{cases} \quad (4.64)$$

Putting these relations to Eq. (4.62), we obtain

$$I = 3 - 2\tau - (\mathcal{C}_{AB}^2 + \mathcal{C}_{AC}^2 + \mathcal{C}_{BC}^2). \quad (4.65)$$

Since τ and \mathcal{C}^2 s are greater than or equal to zero, the union I can assume the maximum value 3 when τ, \mathcal{C}^2 s = 0, for example, in a fully separable state.

From Eq. (4.65), we can see that the union I is related not only to 3-way entanglement (quantified by τ), but also to all 2-way entanglements (quantified by \mathcal{C}^2 s). Thus the union I is a quantity which involves all entanglements of a triqubit qubit state. It is a potential measure of total entanglement for triqubit pure states. From the entanglement Venn diagrams introduced in the preceding section, entanglement of triqubit pure states is more complex than the one of biqubit pure states so that it is impossible to completely quantify

the entanglement of triqubit pure states by only one parameter, such as the squared concurrence \mathcal{C}^2 s or the 3-tangle τ . The union I quantifies the entanglement of a triqubit pure state from the respect of the whole state. That is, the union I answers the question “How much entanglement, including 2- and 3-way entanglements, does a state possess?” Therefore, from the value of the union I of a state, in general, we do not determine the class of the entanglement of the state but know the amount of the total entanglement of the state. The union I can give a definite answer about the class of the entanglement of the state only in the following two extremal cases: the fully separable state when the union I satisfies $I = 3$ and the GHZ state when the union I satisfies $I = 1$.

Now let us discuss triqubit pure states of different entanglements by the union I in detail.

Case 1: fully separable states $\rho \in \{1^3\}$. A triqubit pure state is fully separable if and only if all the three qubits have no entanglement, i.e., no nonlocal reality, $\tau_{i(jk)} = 0$ for $i, j, k \in \{A, B, C\}$, but only single reality, $S_i^2 = 1$ for $i \in \{A, B, C\}$. That is all 2- and 3-way entanglements are zero, i.e., τ, \mathcal{C}^2 s = 0. Thus, by Eq. (4.65), a triqubit pure state is fully separable if and only if its union $I = 3$. Therefore the union $I = 3$ is a necessary and sufficient condition on triqubit fully separable pure states $\rho \in \{1^3\}$.

Case 2: biseparable states $\rho \in \{1^1, 2^1\}$. For triqubit biseparable pure states, for example, states with form $\rho_A \otimes \rho_{BC}$, qubit A has no entanglement (i.e., no nonlocal reality, $\tau_{A(BC)} = 0$, but only single reality, $S_A^2 = 1$) while qubits B and C are entangled with each other, i.e.,

$$\begin{cases} \tau = \mathcal{C}_{AB}^2 = \mathcal{C}_{AC}^2 = 0, \\ 0 < \mathcal{C}_{BC}^2 \leq 1. \end{cases} \quad (4.66)$$

The union I can be written as

$$I = 3 - \mathcal{C}_{BC}^2. \quad (4.67)$$

Combining Eq. (4.66), we obtain the range for the union I of biseparable states as

$$2 \leq I < 3 \quad (4.68)$$

where the lower bound can be achieved by states with maximal bipartite entanglement between two of the three qubits, that is, the product states of one of the Bell states with a single-qubit pure state.

Case 3 : fully entangled states $\rho \in \{3^1\}$. Since the lower bound to the union I for states $\rho \in \{1^1, 2^1\}$ is 2, the unique possibility of states with $I < 2$ is fully entangled. Thus $I < 2$ is a sufficient condition on triqubit fully entangled pure states $\rho \in \{3^1\}$.

Case 3-I: states with W entanglement $\rho \in \{\text{W entanglement}\}$. For example, state $|\Psi\rangle$ with the following wave function

$$|\Psi\rangle = \alpha|100\rangle + \beta|010\rangle + \gamma|001\rangle \quad (4.69)$$

where $\alpha, \beta, \gamma \neq 0$ and $|\alpha|^2 + |\beta|^2 + |\gamma|^2 = 1$. There is no 3-way entanglement, i.e., $\tau = 0$, but three 2-way entanglements, i.e., $0 < \mathcal{C}^2\text{s} \leq 1$. The three 2-way entanglements can be calculated by Eq. (4.69) so that the union I is written as

$$I = 3 - 4(|\alpha\beta|^2 + |\alpha\gamma|^2 + |\beta\gamma|^2) \quad (4.70)$$

With the conditions $\alpha, \beta, \gamma \neq 0$ and $|\alpha|^2 + |\beta|^2 + |\gamma|^2 = 1$, we obtain the range for the union I of states with the W entanglement as

$$\frac{5}{3} \leq I < 3 \quad (4.71)$$

where the lower bound $5/3$ is achieved only by the W state with $\alpha = \beta = \gamma = 1/\sqrt{3}$.

Case 3-II: states with GHZ entanglement $\rho \in \{\text{GHZ entanglement}\}$. For example, state $|\Psi\rangle$ with the following wave function

$$|\Psi\rangle = \alpha|000\rangle + \beta|111\rangle \quad (4.72)$$

where $\alpha, \beta \neq 0$ and $|\alpha|^2 + |\beta|^2 = 1$. There is no 2-way entanglement, i.e., $\mathcal{C}^2\text{s} = 0$, but only 3-way entanglement, i.e., $0 < \tau \leq 1$. Thus the union I can be written as

$$I = 3 - 8|\alpha\beta|^2 \quad (4.73)$$

With the conditions $\alpha, \beta \neq 0$ and $|\alpha|^2 + |\beta|^2 = 1$, we obtain the range for the union I of states with GHZ entanglement as

$$1 \leq I < 3 \quad (4.74)$$

where the lower bound 1 is achieved only by the GHZ state with $\alpha = \beta = 1/\sqrt{2}$.

Case 3-III: states with mixed entanglement $\rho \in \{\text{mixed entanglement}\}$. For example, state $|\Psi\rangle$ with the following wave function

$$|\Psi\rangle = \alpha|000\rangle + \beta|001\rangle + \gamma|100\rangle + \lambda|111\rangle \quad (4.75)$$

where $\alpha, \beta, \gamma, \lambda \neq 0$ and $|\alpha|^2 + |\beta|^2 + |\gamma|^2 + |\lambda|^2 = 1$. There are not only three 2-way entanglements but also 3-way entanglement, simultaneously. With the concrete formulae of all 2- and 3-way entanglements, the union I can be written as

$$I = 3 - 8|\alpha\lambda|^2 - 4(|\beta\gamma|^2 + |\beta\lambda|^2 + |\gamma\lambda|^2). \quad (4.76)$$

Table 4.1: Relations of the union I and triqubit pure states with different entanglements.

States	Range of I	Case of extremum
$\rho \in \{1^3\}$	$I = 3$	fully separable state
$\rho \in \{1^1, 2^1\}$	$2 \leq I < 3$	Bell state \otimes single-qubit state
$\rho \in \{\text{W entanglement}\}$	$5/3 \leq I < 3$	the W state
$\rho \in \{\text{GHZ entanglement}\}$	$1 \leq I < 3$	the GHZ state
$\rho \in \{\text{Mixed entanglement}\}$	$1 < I < 3$	<i>NO</i>

With the conditions $\alpha, \beta, \gamma, \lambda \neq 0$ and $|\alpha|^2 + |\beta|^2 + |\gamma|^2 + |\lambda|^2 = 1$, we obtain the range for the union I of states with the mixed entanglement as

$$1 < I < 3 \quad (4.77)$$

where the union I has no extremal value.

Table (4.1) lists the relations of the union I and triqubit pure states with different entanglements.

In the introduction of entanglement measures, we have listed several requirements for a quantity E to be a good entanglement measure. One of them is the normalization of the measure. Since here we consider only the qubit, a 2-level quantum system, the normalization of the measure can be re-expressed by stating that state ρ is separable if and only if $E(\rho) = 0$ holds and the entanglement of a maximally entangled state is given by $E(\rho^M) = \log_2 2 = 1$.

According to these two conditions, the union I is not a good entanglement measure by its value. We have shown that state ρ is separable if and only if its union $I = 3$ holds; and state ρ is the maximally entangled state if and only if $I = 1$ holds. At the same time, the union I is decreasing with increasing entanglement of the state from Eq. (4.65). Thus we need to introduce a new quantity based on the union I . The new quantity can fulfill the requirements and be a good entanglement measure.

Based on Eq. (4.65), we introduce a quantity, denoted as $\tau^{(T)}$, as

$$\tau^{(T)} \equiv \frac{3 - I}{3 - 1} = \frac{1}{2}(3 - I). \quad (4.78)$$

Invoking an analogy to the names of 3-tangle [83] quantifying 3-way entanglement and the partial tangle [93] quantifying the residual two-qubit entanglement, we call the quantity $\tau^{(T)}$ the total tangle of a triqubit pure state. Combining Eqs. (4.65) and (4.78), the total tangle $\tau^{(T)}$ is written in detail

as

$$\tau^{(T)} = \tau + \frac{1}{2}(\mathcal{C}_{AB}^2 + \mathcal{C}_{AC}^2 + \mathcal{C}_{BC}^2). \quad (4.79)$$

All the conclusions of the union I obtained above can be directly transformed into the ones re-expressed in the term of the total tangle $\tau^{(T)}$. By the value of the total tangle $\tau^{(T)}$, we quantify total entanglement of a triqubit pure state. For example, state ρ is separable if and only if its total tangle $\tau^{(T)} = 0$ holds, and ρ is maximally entangled if and only if its total tangle $\tau^{(T)} = 1$ holds. Similar to the union I , when the value of the total tangle $\tau^{(T)}$ of a state lies in the open interval between 0 and 1, i.e., $\tau^{(T)} \in (0, 1)$, we do not determine the class of the entanglement but the amount of the total entanglement of the state. For example, let us take $\tau^{(T)} = 2/3$, which is equivalent to $I = 5/3$, the state may be the W state, but it can also belong to the GHZ entanglement or to the mixed entanglement.

4.5 Generalization

In the preceding sections, we introduced entanglement Venn diagrams and the union I for triqubit pure states. Note that we would rather use the union I than the total tangle $\tau^{(T)}$ though both are equivalent and can be easily transformed into each other. This is since the union I directly corresponds to set theory and can be understood intuitively.

4.5.1 Interesting bounds

Let us recall quantitative complementarity relations for N -qubit pure states. For a pure state of N qubits A_1, A_2, \dots, A_N , the following quantitative complementarity relations were suggested [34, 35]

$$\tau_{k(R_k)} + S_k^2 = 1 \quad (4.80)$$

where $k = 1, 2, \dots, N$ and R_k denotes the set of the $(N - 1)$ qubits other than qubit A_k . Here $\tau_{k(R_k)}$ quantifies the nonlocal reality of qubit A_k , which measures entanglement between qubits A_k and the remaining $(N - 1)$ qubits. S_k^2 quantifies the local reality, i.e., the single particle property, of qubit A_k .

By quantitative complementarity relations, qubit A_k in an N -qubit pure state is described by two parts, the nonlocal reality $\tau_{k(R_k)}$ and the local reality S_k^2 , where the sum of the two parts, denoted as I_k , is always equal to 1. If qubit A_k is regarded as a subset k composed of two parts, where two parts and the area of subset k correspond to $\tau_{k(R_k)}$, S_k^2 , and I_k of qubit A_k , respectively, then an N -qubit pure state can be regarded as a set of N

subsets. In other words, we can construct a map between a set of N subsets and an N -qubit pure state, where subset k corresponds to qubit A_k , the intersection of subset k with other subsets to entanglement $\tau_{k(R_k)}$ between qubit A_k and the remaining $(N - 1)$ qubits, and the relative complement of the intersection in subset k to the single particle property S_k^2 of qubit A_k .

To put the discussion of entanglement on a more solid basis, we define the union, denoted as I , of an N -qubit pure state, invoking an analogy to set theory, as

$$I \equiv I_1 \cup I_2 \cup \cdots \cup I_N. \quad (4.81)$$

Because of $I_k = 1$ for $k = 1, 2, \cdots, N$, the union I reaches the maximum value N when all qubits are disjoint, for example, in a fully separable state, and the minimum value 1 when all qubits overlap completely, for example, in the N -qubit GHZ state. It is shown in Fig. (4.11) that all N -qubit pure states lie in the ring with radius $1 \leq I \leq N$.

Theorem 1 (Separability Criterion). *An N -qubit pure state is fully separable if and only if its union I is equal to N , i.e.,*

$$I = N. \quad (4.82)$$

Proof. —In set theory, since the area of any subset is 1, the union I of the set composed of N subsets is N if and only if N subsets are disjoint, that is, if there is no intersection among N subsets. According to the map between the set of N subsets and the N -qubit pure state, “there is no intersection among N subsets” means there is no entanglement among N qubits. Therefore an N -qubit pure state is fully separable if and only if its union I satisfies $I = N$. \square

In other words, the union I of an N -qubit pure state satisfies $I < N$ if and only if the qubits intersect, that is, if the state is entangled. It is shown in Fig. (4.11) that all N -qubit fully separable pure states lie on the periphery of the circle with radius $I = N$, while all N -qubit entangled pure states lie in the ring with radius $1 \leq I < N$.

Since the local reality of each qubit in an N -qubit pure state can be obtained, for the purpose of practical operation, the separability criterion can also be presented as: an N -qubit pure state is fully separable if and only if

$$\sum_{k=1}^N S_k^2 = N \quad (4.83)$$

holds, otherwise the state is entangled. For an N -qubit pure state, Eq. (4.83) holds if and only if $S_k^2 = 1$ ($\tau_{k(R_k)} = 0$) for $k = 1, 2, \cdots, N$ hold, i.e., the

state is fully separable. Therefore we can operationally distinguish N -qubit entangled pure states from separable ones by calculating the sum of the local realities of N qubits.

Now consider the partition of N -qubit pure states with the help of partition theory (some applications of partition theory can also be seen in [55, 56, 63]). A partition of N qubits is given by

$$\{1^{r_1}, 2^{r_2}, \dots, i^{r_i}, \dots, N^{r_N}\} \quad (4.84)$$

with $\sum_{i=1}^N i r_i = N$, and the number of parts $k = \sum_{i=1}^N r_i$, where, for example, i^{r_i} , the base i is the number of qubits in the part, the superscript r_i is the number of parts with the same number of qubits.

Here we only consider a special partition of an N -qubit pure state where each part is the minimal composition of qubits, which can not be separated any more without destroying entanglement of the state. That is, we only consider the partition of an N -qubit pure state where either the part consists of a single qubit or all the qubits in one and the same part, suppose $M (> 1)$ qubits, are in an M -qubit fully entangled state so that the entanglement of the N -qubit state would be destroyed if the part were separated any more. For example, for $N = 6$, $\{1^1, 2^1, 3^1\}$ denotes all possible partitions of 6 qubits into 3 parts, where the 3 parts consist of 1, 2 and 3 qubits, respectively. Here consider the part with 2 qubits, the qubits therein are entangled each other, but the part is entirely separable from the other two parts. Note that there may be many partitions that correspond to the same number k of parts which are all called k -partite splits, for example, $\{1^1, 2^1, 3^1\}$, $\{2^3\}$ and $\{1^2, 4^1\}$ are all called 3-partite splits of 6 qubits.

Corollary 2. *For an N -qubit entangled pure state with k -partite splits, where $1 \leq k < N$, the lower bound to the union I is k , i.e.,*

$$k \leq I < N. \quad (4.85)$$

Proof. —For an N -qubit entangled pure state with k -partite splits, if the part consists of only one qubit, its entirety is always equal to 1. If the part consists of more than one qubit, suppose M qubits, its entirety can achieve the lower bound 1 when these M qubits are in the M -qubit GHZ state. Therefore the lower bound to the union I , which is the sum of entireties of the k parts, is k when the entirety of each part reaches its lower bound 1. \square

It is shown in Fig. (4.11) that the N -qubit entangled pure states with k -partite splits lie in the ring with radius $k \leq I < N$, while either the part

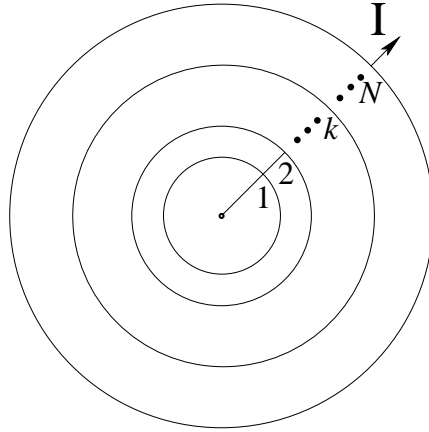


Figure 4.11: Distribution of N -qubit pure states via the amount of the union I .

consists of a single qubit or all the qubits in the part, suppose M qubits, are in the M -qubit GHZ state, the N -qubit state lies on the periphery of the circle with radius $I = k$.

Corollary 3. *An N -qubit entangled pure state with the union $I < 2$ must be fully entangled.*

Proof. —According to Corollary 2, if the union I of an N -qubit pure state satisfies $I < 2$, the number k of the part of the state must be 1. Namely the state with the union $I < 2$ must be a 1-partite split, which can not be separated any more. Therefore an N -qubit pure state with the union $I < 2$ must be fully entangled. \square

Thus $I < 2$ is a sufficient condition on the N -qubit fully entangled pure state. It is shown in Fig. (4.11) that the states, which lie in the ring with radius $1 \leq I < 2$, must be fully entangled.

Because of the complete overlap of all qubits, the N -qubit GHZ state possesses the minimal amount of the union $I = 1$, which lies on the periphery of the circle with radius $I = 1$ in Fig. (4.11).

4.5.2 Detailed formulations

The exact formulations of the measures for N -way entanglement are unknown until now. We cannot formulate the detailed union I and draw an entanglement Venn diagram for an N -qubit pure state as in the case of the triqubit

pure state. But guided by the detailed union I and entanglement Venn diagrams for triqubit pure states, we conjecture a few results for N -qubit pure states.

In a pure state of qubits A , B and C , for example, focusing on qubit A , the nonlocal reality $\tau_{A(BC)}$ of qubit A can be separated into two different kinds of parts. One kind of part is the 3-way entanglement. Another kind of parts are the 2-way entanglements involving qubit A . Consider now a pure state of four qubits A_1 , A_2 , A_3 and A_4 . By analogy with the case of the triqubit pure state, focusing on qubit A_1 , the nonlocal reality $\tau_{A_1(A_2A_3A_4)}$ of qubit A_1 can be separated into three different kinds of parts. The first kind of part is the 4-way entanglement $\tau_{A_1A_2A_3A_4}$. The second kind of parts are the 3-way entanglements $\tau_{A_1A_2A_3}$, $\tau_{A_1A_2A_4}$ and $\tau_{A_1A_3A_4}$ involving qubit A_1 . The third kind of parts are the 2-way entanglements $\mathcal{C}_{A_1A_2}^2$, $\mathcal{C}_{A_1A_3}^2$ and $\mathcal{C}_{A_1A_4}^2$ involving qubit A_1 . Thus we conjecture the following detailed quantitative complementarity relation of qubit A_1 in a 4-qubit pure state:

$$\begin{array}{c}
 \begin{array}{ccc}
 \text{4-way entanglement} & \text{3-way entanglements} & \text{2-way entanglements} \\
 \underbrace{\tau_{A_1A_2A_3A_4}} & + \underbrace{\tau_{A_1A_2A_3} + \tau_{A_1A_2A_4} + \tau_{A_1A_3A_4}} & + \underbrace{\mathcal{C}_{A_1A_2}^2 + \mathcal{C}_{A_1A_3}^2 + \mathcal{C}_{A_1A_4}^2} \\
 \hline
 \text{nonlocal reality} & &
 \end{array} \\
 + \underbrace{S_{A_1}^2}_{\text{local reality}} = 1.
 \end{array} \tag{4.86}$$

Analogous relations also hold for qubits A_2 , A_3 and A_4 .

We show the entanglement Venn diagram for a pure state of four qubits A_1 , A_2 , A_3 and A_4 in Fig. (4.12). By analogy with the case of the triqubit pure state, we consider qubit A_1 as the focus, shown as a bold-faced circle in Fig. (4.12). The relative complement of tripe of qubits $(A_2A_3A_4)$ in qubit A_1 , $A_1|(A_2 \cup A_3 \cup A_4)$, expresses the single-particle property $S_{A_1}^2$ of qubit A_1 . The intersection of qubit A_1 with tripe of qubits $(A_2A_3A_4)$, $A_1 \cap (A_2 \cup A_3 \cup A_4)$, expresses entanglement $\tau_{A_1(A_2A_3A_4)}$, i.e., the nonlocal reality of qubit A_1 . The intersections $(A_1 \cap A_2)|(A_3 \cup A_4)$, $(A_1 \cap A_3)|(A_2 \cup A_4)$ and $(A_1 \cap A_4)|(A_2 \cup A_3)$ express three 2-way entanglements $\mathcal{C}_{A_1A_2}^2$, $\mathcal{C}_{A_1A_3}^2$ and $\mathcal{C}_{A_1A_4}^2$. The intersections $(A_1 \cap A_2 \cap A_3)|A_4$, $(A_1 \cap A_2 \cap A_4)|A_3$ and $(A_1 \cap A_3 \cap A_4)|A_2$ express three 3-way entanglements $\tau_{A_1A_2A_3}$, $\tau_{A_1A_2A_4}$ and $\tau_{A_1A_3A_4}$. The intersection $A_1 \cap A_2 \cap A_3 \cap A_4$ expresses 4-way entanglement $\tau_{A_1A_2A_3A_4}$. The cases of qubits A_2 , A_3 and A_4 are similar to the one of qubit A_1 .

By Fig. (4.12), the union I for a 4-qubit pure state can be written in

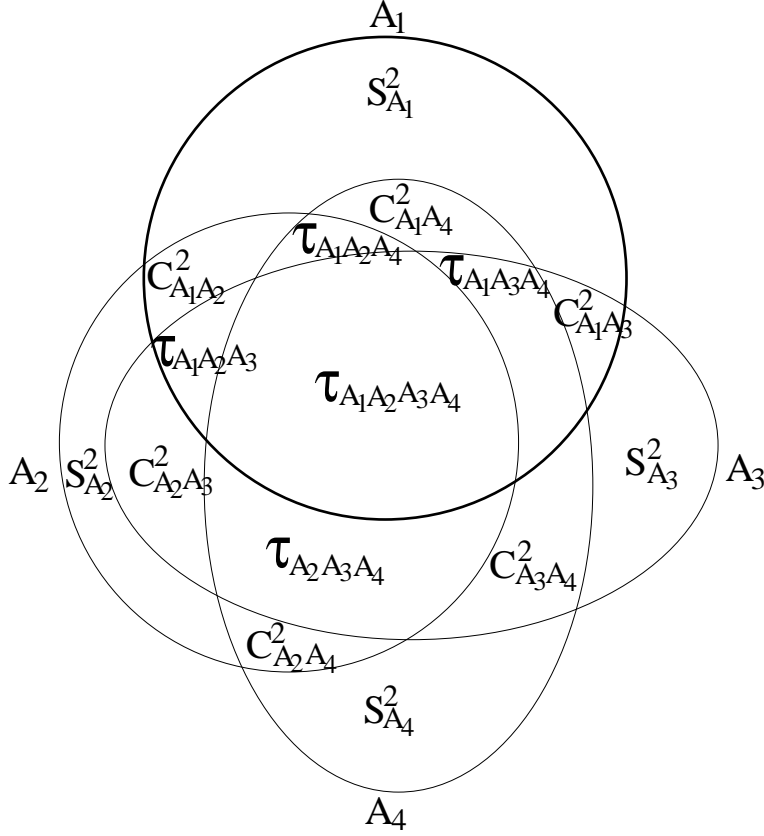


Figure 4.12: Entanglement Venn diagram for a pure state of four qubits A_1 , A_2 , A_3 and A_4 .

detail as

$$\begin{aligned}
 I = & \underbrace{\tau_{A_1 A_2 A_3 A_4}}_{\text{4-way entanglement}} + \underbrace{\tau_{A_1 A_2 A_3} + \tau_{A_1 A_2 A_4} + \tau_{A_1 A_3 A_4} + \tau_{A_2 A_3 A_4}}_{\text{3-way entanglements}} \\
 & + \underbrace{C_{A_1 A_2}^2 + C_{A_1 A_3}^2 + C_{A_1 A_4}^2 + C_{A_2 A_3}^2 + C_{A_2 A_4}^2 + C_{A_3 A_4}^2}_{\text{2-way entanglements}} \\
 & + \underbrace{S_{A_1}^2 + S_{A_2}^2 + S_{A_3}^2 + S_{A_4}^2}_{\text{local realities}}.
 \end{aligned} \tag{4.87}$$

By Eq. (4.86), we have

$$\begin{aligned}
 S_{A_1}^2 = & 1 - \tau_{A_1 A_2 A_3 A_4} - (\tau_{A_1 A_2 A_3} + \tau_{A_1 A_2 A_4} + \tau_{A_1 A_3 A_4}) \\
 & - (C_{A_1 A_2}^2 + C_{A_1 A_3}^2 + C_{A_1 A_4}^2).
 \end{aligned} \tag{4.88}$$

In the same way, we can obtain three similar expressions for $S_{A_2}^2$, $S_{A_3}^2$ and $S_{A_4}^2$. Then we have

$$\begin{aligned}
I = & 4 - 3 \overbrace{\tau_{A_1 A_2 A_3 A_4}}^{\text{4-way entanglement}} - 2 \overbrace{(\tau_{A_1 A_2 A_3} + \tau_{A_1 A_2 A_4} + \tau_{A_1 A_3 A_4} + \tau_{A_2 A_3 A_4})}^{\text{3-way entanglements}} \\
& - \overbrace{(\mathcal{C}_{A_1 A_2}^2 + \mathcal{C}_{A_1 A_3}^2 + \mathcal{C}_{A_1 A_4}^2 + \mathcal{C}_{A_2 A_3}^2 + \mathcal{C}_{A_2 A_4}^2 + \mathcal{C}_{A_3 A_4}^2)}^{\text{2-way entanglements}}.
\end{aligned} \tag{4.89}$$

The total tangle $\tau^{(T)}$ for a 4-qubit pure state can be written as

$$\begin{aligned}
\tau^{(T)} &= \frac{4 - I}{4 - 1} \\
&= \overbrace{\tau_{A_1 A_2 A_3 A_4}}^{\text{4-way entanglement}} + \frac{2}{3} \overbrace{(\tau_{A_1 A_2 A_3} + \tau_{A_1 A_2 A_4} + \tau_{A_1 A_3 A_4} + \tau_{A_2 A_3 A_4})}^{\text{3-way entanglements}} \\
&\quad + \frac{1}{3} \overbrace{(\mathcal{C}_{A_1 A_2}^2 + \mathcal{C}_{A_1 A_3}^2 + \mathcal{C}_{A_1 A_4}^2 + \mathcal{C}_{A_2 A_3}^2 + \mathcal{C}_{A_2 A_4}^2 + \mathcal{C}_{A_3 A_4}^2)}^{\text{2-way entanglements}}.
\end{aligned} \tag{4.90}$$

Consider two typical 4-qubit pure states, the 4-qubit GHZ state and the 4-qubit W state. For the 4-qubit GHZ state

$$|\text{GHZ}\rangle_4 = \frac{1}{\sqrt{2}}(|0000\rangle + |1111\rangle), \tag{4.91}$$

there is no 2- and 3-way entanglement but only a 4-way entanglement with the maximum 1, i.e.,

$$\begin{cases} \tau_X = 1 & \text{for } X = A_1 A_2 A_3 A_4; \\ \tau_X = 0 & \text{for others.} \end{cases} \tag{4.92}$$

The total tangle $\tau^{(T)}$ of the state is

$$\tau^{(T)} = \tau_{A_1 A_2 A_3 A_4} = 1. \tag{4.93}$$

For the 4-qubit W state

$$|\text{W}\rangle_4 = \frac{1}{2}(|1000\rangle + |0100\rangle + |0010\rangle + |0001\rangle), \tag{4.94}$$

there is no 3- and 4-way entanglement but only six 2-way entanglements. These six 2-way entanglements are given in [31] as

$$\mathcal{C}_{A_i A_j}^2 = \frac{1}{4} \tag{4.95}$$

for $A_i, A_j \in \{A_1, A_2, A_3, A_4\}$. Then the total tangle $\tau^{(T)}$ is

$$\tau^{(T)} = \frac{1}{3}(\mathcal{C}_{A_1A_2}^2 + \mathcal{C}_{A_1A_3}^2 + \mathcal{C}_{A_1A_4}^2 + \mathcal{C}_{A_2A_3}^2 + \mathcal{C}_{A_2A_4}^2 + \mathcal{C}_{A_3A_4}^2) = \frac{1}{2}. \quad (4.96)$$

Now consider a pure state of N qubits A_1, A_2, \dots, A_N . We introduce a quantity $\tau_{A_i}^{(m)}$ which is defined as the sum of all m -way entanglements related with qubit A_i as

$$\tau_{A_i}^{(m)} \equiv \underbrace{\tau_{A_i \dots A_m}}_m + \dots + \underbrace{\tau_{A_i \dots A_N}}_m. \quad (4.97)$$

For example, $N = 4$,

$$\begin{cases} \tau_{A_i}^{(2)} = \tau_{A_i A_j} + \tau_{A_i A_k} + \tau_{A_i A_l}, \\ \tau_{A_i}^{(3)} = \tau_{A_i A_j A_k} + \tau_{A_i A_j A_l} + \tau_{A_i A_k A_l}, \\ \tau_{A_i}^{(4)} = \tau_{A_i A_j A_k A_l}, \end{cases} \quad (4.98)$$

for $A_i, A_j, A_k, A_l \in \{A_1, A_2, A_3, A_4\}$. Here we substitute $\tau_{A_i A_j}$ for $\mathcal{C}_{A_i A_j}^2$ to denote the squared concurrence between qubits A_i and A_j . Because the local reality $S_{A_i}^2$ quantifies the single-partite property of qubit A_i , by analogy with the m -way entanglement, we can call the single-partite property $S_{A_i}^2$ the 1-way entanglement, denoted as $\tau_{A_i}^{(1)}$, of qubit A_i . Of course, the 1-way entanglement $\tau_{A_i}^{(1)}$ is not true entanglement at all. That is, we substitute $\tau_{A_i}^{(1)}$ for $S_{A_i}^2$ to denote the local reality of qubit A_i . Then the quantitative complementarity relation for qubit A_i in an N -qubit pure state can be written, as speculated in [35], as

$$\sum_{m=1}^N \tau_{A_i}^{(m)} = \underbrace{\tau_{A_i}^{(1)}}_{\text{local reality}} + \underbrace{\tau_{A_i}^{(2)} + \dots + \tau_{A_i}^{(N)}}_{\text{nonlocal realities}} = 1 \quad (4.99)$$

where $\tau_{A_i}^{(1)}$ is related with the local reality of qubit A_i while all the others are related with the nonlocal realities of qubit A_j .

We also introduce another quantity $\tau^{(m)}$ which is defined as the sum of all m -way entanglements in the state as

$$\tau^{(m)} \equiv \tau_{A_1 A_2 \dots A_m} + \dots + \tau_{A_{(N+1-m)} \dots A_N}. \quad (4.100)$$

For example, $N = 4$,

$$\begin{cases} \tau^{(2)} = \tau_{A_i A_j} + \tau_{A_i A_k} + \tau_{A_i A_l} + \tau_{A_j A_k} + \tau_{A_j A_l} + \tau_{A_k A_l}, \\ \tau^{(3)} = \tau_{A_i A_j A_k} + \tau_{A_i A_j A_l} + \tau_{A_i A_k A_l} + \tau_{A_j A_k A_l}, \\ \tau^{(4)} = \tau_{A_i A_j A_k A_l}, \end{cases} \quad (4.101)$$

for $A_i, A_j, A_k, A_l \in \{A_1, A_2, A_3, A_4\}$. The definition (4.100) also holds for the 1-way entanglements (i.e., the local realities) as

$$\tau^{(1)} = \tau_{A_1}^{(1)} + \tau_{A_2}^{(1)} + \cdots + \tau_{A_N}^{(1)} = \sum_{i=1}^N \tau_{A_i}^{(1)}. \quad (4.102)$$

From the definitions of $\tau_{A_i}^{(m)}$ and $\tau^{(m)}$ for an N -qubit pure state, we have the following relation

$$\tau^{(m)} = \frac{1}{m} \sum_{i=1}^N \tau_{A_i}^{(m)}. \quad (4.103)$$

For example, $N = 4$ and $m = 2$,

$$\begin{aligned} \sum_{i=1}^4 \tau_{A_i}^{(2)} &= \tau_{A_1}^{(2)} + \tau_{A_2}^{(2)} + \tau_{A_3}^{(2)} + \tau_{A_4}^{(2)} \\ &= 2(\tau_{A_1 A_2} + \tau_{A_1 A_3} + \tau_{A_1 A_4} + \tau_{A_2 A_3} + \tau_{A_2 A_4} + \tau_{A_3 A_4}) \\ &= 2\tau^{(2)}. \end{aligned} \quad (4.104)$$

By the definition of the union I for an N -qubit pure state in Eq. (4.81), we can write the detailed union I as

$$I = \sum_{m=1}^N \tau^{(m)} = \underbrace{\tau^{(1)}}_{\text{local realities}} + \underbrace{\sum_{m=2}^N \tau^{(m)}}_{\text{nonlocal realities}}. \quad (4.105)$$

From the viewpoint of characterization of entanglement in the N -qubit pure state, the local realities $\tau^{(1)}$ are unwanted terms in the union I . By Eq. (4.99), we have

$$\tau_{A_i}^{(1)} = 1 - \sum_{m=2}^N \tau_{A_i}^{(m)}. \quad (4.106)$$

Combining Eqs. (4.102) and (4.103), we have

$$\begin{aligned} \tau^{(1)} &= N - \sum_{i=1}^N \sum_{m=2}^N \tau_{A_i}^{(m)} \\ &= N - \sum_{m=2}^N m\tau^{(m)}. \end{aligned} \quad (4.107)$$

Thus

$$\begin{aligned} I &= N - \sum_{m=2}^N m\tau^{(m)} + \sum_{m=2}^N \tau^{(m)} \\ &= N - \sum_{m=2}^N (m-1)\tau^{(m)}. \end{aligned} \quad (4.108)$$

The total tangle $\tau^{(T)}$ for an N -qubit pure state can be written as

$$\begin{aligned} \tau^{(T)} &= \frac{N-I}{N-1} \\ &= \frac{1}{N-1} \sum_{m=2}^N (m-1)\tau^{(m)}. \end{aligned} \quad (4.109)$$

For the N -qubit GHZ state

$$|\text{GHZ}\rangle_N = \frac{1}{\sqrt{2}}(|00\cdots 0\rangle + |11\cdots 1\rangle), \quad (4.110)$$

there is no entanglement but only an N -way entanglement with the maximum 1, i.e.,

$$\begin{cases} \tau^{(N)} = 1, \\ \tau^{(m)} = 0 \quad \text{for } 1 \leq m < N. \end{cases} \quad (4.111)$$

The total tangle $\tau^{(T)}$ is given by

$$\tau^{(T)} = \tau^{(N)} = 1. \quad (4.112)$$

For the N -qubit W state

$$|\text{W}\rangle_N = \frac{1}{\sqrt{N}}(|10\cdots 0\rangle + |01\cdots 0\rangle + \cdots + |00\cdots 1\rangle), \quad (4.113)$$

there is only the 2-way entanglements which are given by [31]

$$\tau_{A_i A_j} = \frac{4}{N^2} \quad (4.114)$$

for $i, j \in \{1, 2, \dots, N\}$. There are $(N(N-1)/2)$ 2-way entanglements in the N -qubit W state. Then we have

$$\tau^{(2)} = \frac{N(N-1)}{2} \cdot \frac{4}{N^2} = \frac{2(N-1)}{N}. \quad (4.115)$$

Thus the total tangle $\tau^{(T)}$ is written as

$$\tau^{(T)} = \frac{1}{N-1} \tau^{(2)} = \frac{2}{N}. \quad (4.116)$$

Chapter 5

Multiparticle Entanglement

In the preceding chapter, we have discussed quantum systems in which the Hilbert-space dimensions of all particles are the same and equal to 2, such as spin-1/2 particles, so that each particle can be regarded as a qubit.

In this chapter, we will discuss quantum systems where the particles have arbitrary Hilbert-space dimensions. That is, in a quantum system which will be discussed in this chapter, the Hilbert-space dimension of the particle can be any positive integer greater than 1, and different particles can have different Hilbert-space dimensions. For simplicity, we omit the words “multiparticle arbitrary-dimensional” in the following part of this chapter. Another important difference from the preceding chapter is that in this chapter we will use the ranks of the (reduced) density matrices of the states as the tool to characterize entanglement of the states. In this chapter, we will focus on the following two questions. One is the first task of characterizing entanglement: “is a state entangled or not?”, i.e., detection of entanglement. Another is one subtask of the second task of characterizing entanglement: “is a state of several subsystems entangled or not?”.

This chapter is organized as follows: In section 1, we discuss the case of pure states. We propose two necessary and sufficient conditions for entangled and fully entangled pure states, respectively. Then we present a procedure to find a special partition, which has been mentioned in the preceding chapter, of a given quantum systems where every part of the special partition contains either $X(> 1)$ fully entangled particles or only a single particle. In section 2, we discuss the case of mixed states. We propose necessary conditions for the separability of mixed states, which naturally lead us to obtain a sufficient condition for entanglement of the states. In a similar way we propose necessary conditions to determine the separability properties of the partitions of all particles in a given mixed state based on hierarchic relations among all possible partitions of the particles.

For convenience, we will use the following notation in this chapter. For a state ρ of N particles A_1, A_2, \dots, A_N , the reduced density matrix obtained by tracing ρ over particle A_i is written as

$$\rho_{R(i)} = \text{Tr}_{A_i}(\rho) \quad (5.1)$$

where $R(i)$ denotes the set of the remaining $(N - 1)$ particles other than particle A_i . The reduced density matrix obtained by tracing ρ over particles A_i and A_j is denoted as

$$\rho_{R(i,j)} = \text{Tr}_{A_j}(\rho_{R(i)}) = \text{Tr}_{A_j}(\text{Tr}_{A_i}(\rho)). \quad (5.2)$$

Here the sequence of tracing particles A_i and A_j over the initial state ρ doesn't influence the final result, i.e.,

$$\rho_{R(i,j)} = \text{Tr}_{A_j}(\text{Tr}_{A_i}(\rho)) = \text{Tr}_{A_i}(\text{Tr}_{A_j}(\rho)). \quad (5.3)$$

In the same way,

$$\rho_{R(i,j,k)} = \text{Tr}_{A_i}(\text{Tr}_{A_j}(\text{Tr}_{A_k}(\rho))), \quad (5.4)$$

and so on. In view of these successive relations, ρ can be called 1-level-higher density matrix of $\rho_{R(i)}$ and 2-level-higher density matrix of $\rho_{R(i,j)}$; $\rho_{R(i)}$ can be called 1-level-higher density matrix of $\rho_{R(i,j)}$ and 2-level-higher density matrix of $\rho_{R(i,j,k)}$; and so on.

It is obvious that the number of the 1-level-higher density matrices of a reduced density matrix can be greater than 1. And a density matrix can be the 1-level-higher density matrix of several different reduced density matrices. For example, the 1-level-higher density matrices of $\rho_{R(i,j)}$ are $\rho_{R(i)}$ and $\rho_{R(j)}$. At the same time, the reduced density matrix $\rho_{R(i,j)}$ is the 1-level-higher density matrix of the reduced density matrices $\rho_{R(i,j,k)}$, $\rho_{R(i,j,l)}$, $\rho_{R(i,j,m)}$, and so on.

In an N -particle state, a density matrix of M ($1 \leq M \leq N$) particles has $(N - M)$ 1-level-higher density matrices and is the 1-level-higher density matrix of M (NOT including the case of $M = 1$) reduced density matrices. If the density matrix contains only 1 ($M = 1$) particles, it is impossible that such density matrix is the 1-level-higher density matrix of some density matrix because such density matrix cannot be traced any more. In Fig. (5.1), a state ρ of three particles A , B and C is taken as the example to show these successive relations.

5.1 Pure states

In this section, we will discuss entanglement of pure states based on the ranks of the (reduced) density matrices. Thus it is necessary to consider the definition of the rank of a matrix.

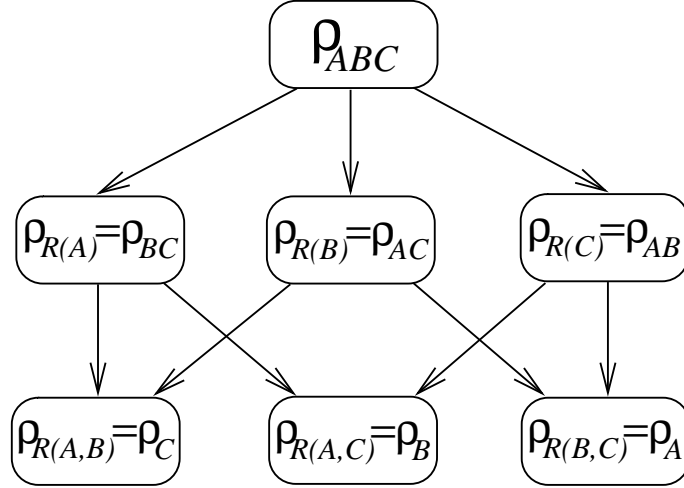


Figure 5.1: Successive relations among (reduced) density matrices of a state ρ with three particles A , B and C . For two density matrices at the two ends of each arrow, the density matrix at the starting point of the arrow is a 1-level-higher density matrix of the density matrix at the end point.

The rank of a matrix ρ , denoted as $rank(\rho)$, is defined as the maximal number of linearly independent row vectors (also column vectors) in the matrix ρ .

It is clear from this definition that

$$0 \leq rank(\rho) \leq \min\{m, n\} \quad (5.5)$$

where m (n) is the number of rows (columns) in the matrix ρ . Here $rank(\rho) = 0$ holds if and only if ρ is the zero matrix.

According to this definition, the rank of the density matrix of a pure state has the following basic property:

Lemma 4. *A state is pure if and only if the rank of its density matrix ρ is equal to 1, i.e.,*

$$rank(\rho) = 1. \quad (5.6)$$

Proof. —A state ρ is pure if and only if $\rho^2 = \rho$ holds, that is, ρ is a projection operator onto a one-dimensional subspace so that only one eigenvalue is equal to 1, all the other ones being zero. Thus the number of linearly independent row vectors of ρ is equal to 1. Therefore $rank(\rho) = 1$ holds for a pure state ρ .

Conversely, for a density matrix ρ with $rank(\rho) = 1$, since there is only one linearly independent row vector of ρ , it is possible to rewrite the density

matrix in a new form with only one element, whose value is equal to 1, by selecting a suitable basis. In that basis, $\rho^2 = \rho$ is evident and hence ρ is pure. \square

5.1.1 Entanglement and full entanglement

Based on this basic property, a necessary and sufficient condition for a pure state to be entangled is obtained as follows.

Lemma 5. *A pure state is entangled if and only if the rank of at least one of its reduced density matrices is greater than 1.*

Proof. —If a pure state is entangled, according to Schrödinger’s definition of entanglement: “The whole is in a definite state, the parts taken individually are not”, then at least one of the states obtained by tracing the original state over some particles is mixed. By Lemma 4, the rank of this reduced state is greater than 1. Conversely, if the rank of one reduced density matrix of a pure state is greater than 1, then the reduced state is mixed, and according to Schrödinger’s definition, the original state is entangled. \square

From Lemma 5 it is obvious that a pure state is entangled if and only if at least one reduced state of the original state is mixed. Of course, an entangled pure state can have more than one mixed reduced states. For example, both reduced density matrices of state $|\Psi\rangle = (1/\sqrt{2})(|01\rangle - |10\rangle)$ (one of the Bell states) are mixed.

An important subclass of the multiparticle entangled states are the so-called fully entangled states [60, 61], which cannot be reduced to mixtures of states where a smaller number of particles are entangled. For example, triqubit states that are not of the forms $\rho_1 \otimes \rho_{23}$, $\rho_2 \otimes \rho_{13}$, and $\rho_3 \otimes \rho_{12}$, or mixtures of these states are fully entangled, such as the GHZ state. In terms of the ranks of reduced density matrices, we obtain the following necessary and sufficient condition for a pure state to be fully entangled:

Theorem 6. *A pure state is fully entangled if and only if the ranks of its all reduced density matrices are greater than 1.*

Proof. —A pure state is fully entangled if and only if every particle and every multi-particle combination in the system are entangled with the remaining particles. That is, the states of every individual particle and every individual multi-particle combination are mixed, i.e., the ranks of all reduced density matrices are greater than 1, and vice versa. \square

An N -particle pure state has

$$\sum_{n=1}^{N-1} \frac{N!}{n!(N-n)!} = 2^N - 2 \quad (5.7)$$

reduced density matrices. Thus a pure state is fully entangled if and only if its all $(2^N - 2)$ reduced density matrices are mixed.

If at least one (but not all) of the reduced states is pure, then the initial entangled state is partially entangled but not fully entangled. That is, for a given entangled pure state, if the rank of at least one reduced density matrix is equal to 1, then one or some of all particles in the state are separable from the remaining particles. This problem will be discussed in the next subsection.

5.1.2 Classification

As mentioned in Chapter 2, one subtask of classification of multipartite entanglement is to determine the separability of the state with respect to partitions. That is, for a given entangled pure state, which particles are entangled with each other? In this subsection, we will present a simple procedure to determine the type of entanglement. In this procedure, we separate all the particles in a given pure state of N particles, without destroying entanglement of the initial state, into the parts of a special partition, where every part contains either X ($1 < X \leq N$) fully entangled particles or only a single particle.

For a given pure state ρ , if its particles are separated into two parts U and V , then the Schmidt decomposition of state ρ is written as

$$\rho = \sum_{i=1}^k \lambda_i |u_i\rangle\langle u_i| \otimes |v_i\rangle\langle v_i| \quad (5.8)$$

where $|u_i\rangle \in \mathcal{H}_U$, $|v_i\rangle \in \mathcal{H}_V$ and $\sum_{i=1}^k \lambda_i = 1$ with $\lambda_i > 0$. Here the number k is called the Schmidt rank of ρ , which is the rank of the reduced density matrix ρ_U (and ρ_V):

$$\text{rank}(\rho_U) = \text{rank}(\rho_V). \quad (5.9)$$

Thus if a pure state has one pure (or mixed) reduced state, then the state has at least two pure (or mixed) reduced states. Then we obtain the following useful Lemma:

Lemma 7. *Given a pure state ρ , if its particles are separated into two parts U and V , then $\text{rank}(\rho_U) = 1$ holds if and only if these two parts are separable, i.e.,*

$$\rho = \rho_U \otimes \rho_V. \quad (5.10)$$

Proof. —If $\text{rank}(\rho_U) = 1$ holds, then $\text{rank}(\rho_V) = 1$ holds by Eq. (5.9), thus states ρ_U and ρ_V are pure by Lemma 4. According to the proposition in Ref. [132]: “For two systems U and V , whenever U is in a pure state, no correlation exists between U and V ”, states ρ_U and ρ_V are separable. Therefore the whole pure state ρ can be written as $\rho = \rho_U \otimes \rho_V$.

Conversely, if ρ is pure and separable with respect to the two parts U and V , that is, $\rho = \rho_U \otimes \rho_V$, then the ranks obey (see, e.g., [133])

$$\text{rank}(\rho) = \text{rank}(\rho_U) * \text{rank}(\rho_V) = 1, \quad (5.11)$$

and hence $\text{rank}(\rho_U) = \text{rank}(\rho_V) = 1$. □

Using the results obtained above, we construct the following procedure to find a special partition of a given pure state ρ of N particles A_1, A_2, \dots, A_N , where each part is the minimal set of particles which cannot be separated any more without destroying entanglement of the initial state, so that the particles are separable when they are in different parts but entangled when they are in one and the same part. Our procedure consists in successively searching for all subsets of growing size which are separable from the rest of the system in the sense of Lemma 7. The maximal set size which has to be checked for separability is $\lfloor N/2 \rfloor$ (the maximal integer less than or equal to $N/2$), since along with every separable set of size M , its complement of size $(N - M)$ also is of course separable from all other particles according to Lemma 7. In more detail the procedure works as follows:

Step 1. Calculate the rank of $\rho_{R(i)}$ for all particles. By Lemma 7, if $\text{rank}(\rho_{R(i)}) = 1$ holds, then ρ factorizes as $\rho = \rho_{A_i} \otimes \rho_{R(i)}$. Suppose there exist M_1 , $0 \leq M_1 \leq N$, particles that satisfy $\text{rank}(\rho_{R(i)}) = 1$, then ρ is the tensor product of M_1 single-particle parts and a part of $(N - M_1)$ particles. After this step, it is impossible that there exists a separable single particle in the $(N - M_1)$ -particle part. Thus if $(N - M_1) \leq 3$ holds, then the procedure ends since the $(N - M_1)$ -particle part cannot contain further separable subsets; otherwise, i.e., if $(N - M_1) > 3$ holds, we perform the next step.

Step 2. For the part of the remaining N_2 , $N_2 = N - M_1$, particles, calculate the rank of $\rho_{R(i,j)}$ for all two-particle combinations. If there exist M_2 , $0 \leq M_2 \leq \lfloor N_2/2 \rfloor$, two-particle combinations that satisfy $\text{rank}(\rho_{R(i,j)}) = 1$, then the part of N_2 particles is the tensor product of M_2 two-particle parts and a part of $(N_2 - 2M_2)$ particles. If $(N_2 - 2M_2) \leq 5$ holds, the

procedure ends since all separable single particle and 2-particle combinations have already been found in these two steps. Otherwise, i.e., if $(N_2 - 2M_2) > 5$ holds, we perform the next step.

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Step X . Following the preceding steps, for the part of N_X , $N_X = N - \sum_{i=1}^{X-1} (i * M_i)$, particles, calculate the rank of $\rho_{R(X)}$ for all X -particle combinations in these N_X particles, where for a certain X -particle combination, $R(X)$ denotes the set of the remaining $(N_X - X)$ particles other than the particles in this combination. If there exist M_X , $0 \leq M_X \leq \lfloor N_X/X \rfloor$, X -particle combinations that satisfy $\text{rank}(\rho_{R(X)}) = 1$, then the part of N_X particles is written as the tensor product of M_X X -particle parts and a part of $(N_X - X * M_X)$ particles. In a similar consideration in the preceding steps, if $(N_X - X * M_X) \leq (2X + 1)$ holds, the $(N_X - X * M_X)$ -particle part cannot contain further separable subsets since all separable x -particle, $x \leq X$, combinations have already been found by assumption, then the procedure ends. Otherwise, i.e., if $(N_X - X * M_X) > (2X + 1)$ holds, we perform the next step.

The following steps are similar to step X . In the end, if we obtain separable parts in the procedure, then state ρ can be written as the tensor product of those parts. If we do not obtain any separable part in the procedure, then state ρ is fully entangled.

As an example to explain the procedure in detail, we use the following six-qubit pure state

$$|\Psi\rangle = \frac{1}{2}(|000000\rangle + |000111\rangle + |011000\rangle + |011111\rangle). \quad (5.12)$$

- Step 1. Calculating $\text{rank}(\rho_{R(i)})$ for all qubits:

$$\text{rank}(\rho_{R(1)}) = 1 \implies \rho = \rho_{A_1} \otimes \rho_{R(1)}. \quad (5.13)$$

Since $(6 - 1) > 3$, we continue.

- Step 2. Calculating $\text{rank}(\rho_{R(i,j)})$ for all 2-qubit combinations in the part of the remaining 5 qubits:

$$\text{rank}(\rho_{R(2,3)}) = 1 \implies \rho_{R(1)} = \rho_{(A_2, A_3)} \otimes \rho_{R(1,2,3)}. \quad (5.14)$$

Since $(5 - 2) < 5$, we end the procedure.

In the end, state ρ can be written as

$$\rho = \rho_{A_1} \otimes \rho_{(A_2, A_3)} \otimes \rho_{(A_4, A_5, A_6)}. \quad (5.15)$$

This procedure is shown in Fig. (5.2) as a tree.

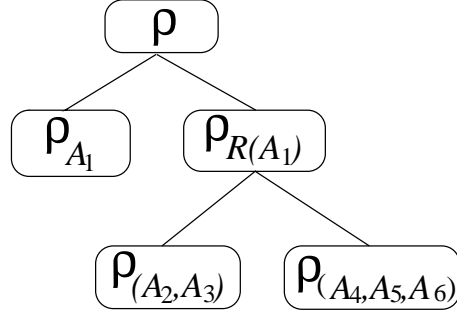


Figure 5.2: Tree form of the procedure of the six-qubit pure state $|\Psi\rangle = (1/2)(|000000\rangle + |000111\rangle + |011000\rangle + |011111\rangle)$. In the diagram, all parts which consist of no subpart are the minimal nonseparable sets of qubits so that the initial state is written as the tensor product of all these parts $\rho = \rho_{A_1} \otimes \rho_{(A_2, A_3)} \otimes \rho_{(A_4, A_5, A_6)}$.

5.2 Mixed states

In this section, we focus on entanglement of mixed states.

5.2.1 Separability of states

In terms of the ranks of reduced density matrices, we obtain the following necessary conditions for separable states:

Theorem 8. *If a state ρ of N particles A_1, A_2, \dots, A_N is separable, then the rank of any reduced density matrix of ρ must be less than or equal to the ranks of all of its 1-level-higher density matrices, i.e.,*

$$\text{rank}(\rho_{R(i)}) \leq \text{rank}(\rho) \quad (5.16)$$

holds for any $A_i \in \{A_1, A_2, \dots, A_N\}$; and

$$\begin{cases} \text{rank}(\rho_{R(i,j)}) \leq \text{rank}(\rho_{R(i)}) \\ \text{rank}(\rho_{R(i,j)}) \leq \text{rank}(\rho_{R(j)}) \end{cases} \quad (5.17)$$

holds for any pair of all particles; and so on.

Proof. —For simplicity, here we only prove (5.16). The remaining inequalities can be proved in a similar way.

A separable mixed state ρ of N particles A_1, A_2, \dots, A_N and its reduced density matrix $\rho_{R(i)}$ can be written as

$$\left\{ \begin{array}{l} \rho = \sum_{j=1}^M p_j \rho^j = \sum_{j=1}^M p_j \bigotimes_{i=1}^N \rho_{A_i}^j \\ \rho_{R(i)} = \sum_{j=1}^M p_j \rho_{R(i)}^j = \sum_{j=1}^M p_j \bigotimes_{\substack{k=1 \\ k \neq i}}^N \rho_{A_k}^j \end{array} \right. \quad (5.18)$$

According to Lemma 4, any pure state can be considered a basis vector in its vector space. Thus M pure states ρ^j , where $\rho^j = \bigotimes_{i=1}^N \rho_{A_i}^j \in \bigotimes_{i=1}^N \mathcal{H}_{A_i}$ for $j = 1, 2, \dots, M$, are M basis vectors that span a vector space $U \subset \bigotimes_{i=1}^N \mathcal{H}_{A_i}$. Here \mathcal{H}_{A_i} denotes the Hilbert space of particle A_i . The maximal number of linearly independent vectors among these M basis vectors is the rank of ρ , $rank(\rho)$, and at the same time, it is the dimension of vector space U .

In a similar way, M basis vectors $\rho_{R(i)}^j$, where $\rho_{R(i)}^j = \bigotimes_{\substack{k=1 \\ k \neq i}}^N \rho_{A_k}^j \in \bigotimes_{\substack{k=1 \\ k \neq i}}^N \mathcal{H}_{A_k}$ for $j = 1, 2, \dots, M$, span a vector space $V \subset \bigotimes_{\substack{k=1 \\ k \neq i}}^N \mathcal{H}_{A_k}$ with the dimension $rank(\rho_{R(i)})$.

From the construction of the vector spaces U and V it is clear that V is a linear subspace of U , and hence its dimension is not greater than that of U . This proves (5.16) since the dimensions of the vector spaces are equal to the ranks of the density matrices. \square

The separability conditions (5.16,5.17) for mixed states are not sufficient. For example, an important family of the biqubit mixed states are the so called Werner states [13], which are mixtures of a maximally entangled biqubit pure state and the separable biqubit maximally mixed state. These states are fully characterized by the fidelity F , which measures the overlap of the maximally entangled biqubit pure state with the Werner states. Though the Werner states do satisfy the separability conditions (5.16,5.17), they are entangled for $F > 1/2$.

The necessary (but not sufficient) conditions (5.16,5.17) for a mixed state to be separable are logically equivalent to the following sufficient (but not necessary) conditions for a mixed state to be entangled:

Corollary 9. *Given a mixed state ρ , if the rank of at least one of the reduced density matrices of ρ is greater than the rank of one of its 1-level-higher density matrices, then the state ρ is entangled.*

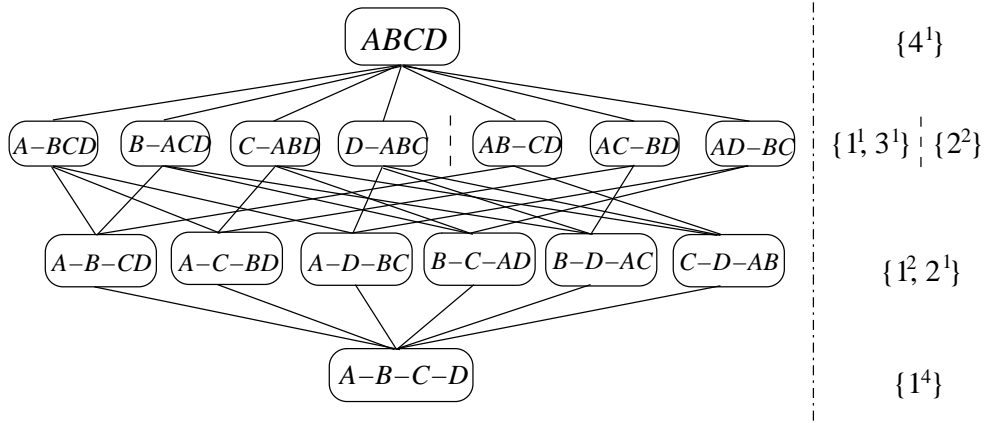


Figure 5.3: Hierarchic relations among all possible partitions of four particles A , B , C and D . The five different kinds of partitions are listed on right side of the figure.

5.2.2 Separability with respect to partitions

For a given mixed state, there are hierarchic relations among all possible partitions of the particles (e.g. in Ref. [55, 56]). For example, consider a partition of all particles into i parts. If we allow some of the parts to act together as a new composite part, then we obtain a new partition into j parts with $j < i$. In Fig. (5.3), we take a state of four particles A , B , C and D as an example to show the hierarchic relations among all possible partitions of the particles.

In a way similar to the proof of the separability conditions (5.16,5.17), we obtain the following interesting separability properties of the partitions of the particles in a given mixed state:

Corollary 10. *Consider a mixed state $\rho = \sum_{j=1}^M p_j \rho^j$ and a partition of the particles. If any two parts U and V in the partition are separable, that is, the state of the composition $(U + V)$ of parts U and V can be written as*

$$\rho_{(U+V)} = \sum_{j=1}^M p_j \rho_{(U+V)}^j = \sum_{j=1}^M p_j (\rho_U^j \otimes \rho_V^j) \quad (5.19)$$

where $\rho_U^j \in \mathcal{H}_U$, $\rho_V^j \in \mathcal{H}_V$ and $\rho_{(U+V)}^j \in \mathcal{H}_{(U+V)}$, then the ranks of the two reduced density matrices ρ_U and ρ_V both are less than or equal to the rank of $\rho_{(U+V)}$, i.e.,

$$\begin{cases} \text{rank}(\rho_U) \leq \text{rank}(\rho_{(U+V)}) \\ \text{rank}(\rho_V) \leq \text{rank}(\rho_{(U+V)}) \end{cases} \quad (5.20)$$

The M basis vectors ρ_U^j and the M basis vectors ρ_V^j span two linear subspaces of the composite vector space spanned by the M basis vectors $\rho_{(U+V)}^j$. Thus as the dimensions of the two linear subspaces, $\text{rank}(\rho_U)$ and $\text{rank}(\rho_V)$ both are not greater than $\text{rank}(\rho_{(U+V)})$, the dimension of the composite vector space, Corollary 10 is proved. The Werner states again show that the separability conditions for mixed states in Corollary 10 are not sufficient.

The necessary separability conditions for the partitions in Corollary 10 can again be reformulated as sufficient entanglement conditions of the partitions: given a mixed state and a partition of the particles, consider any two parts in the partition. If the rank of at least one of the reduced density matrices of the two parts is greater than the rank of the density matrix of the composition of these two parts, then these two parts are entangled.

Chapter 6

Conclusion and Outlook

The characterization, including detection, classification and quantification, of entanglement is perhaps the most challenging open problem of modern quantum theory. Several aspects of this problem have been discussed in this thesis and some interesting results have been obtained for understanding entanglement.

Summing up, the results obtained in this thesis are listed as follows:

- Mixed entanglement of triqubit pure states. Taking the squared concurrence and the 3-tangle as measures of 2- and 3-way entanglement, we proposed a special true tripartite entanglement, the mixed entanglement, which possesses properties of both GHZ entanglement and W entanglement, simultaneously. There exist two inequivalent kinds of sets of four non-superfluous basis vectors for constructing states with mixed entanglement. With one of the two sets, we discussed Walther, Resch and Zeilinger's experiment [94] and contributed to the clarification of its nature.
- Entanglement Venn diagrams for triqubit pure states. Based on quantitative complementarity relations for triqubit pure states, we drew an entanglement Venn diagram for such states to intuitively illustrate entanglement among the three qubits. Then we showed different entanglement Venn diagrams for triqubit pure states with different entanglements. These diagrams helped us obtain a clear picture of the relations among the three qubits in different entanglements.
- Union I (total tangle $\tau^{(T)}$) for quantifying total entanglement of a triqubit pure state. By the entanglement Venn diagram, we introduced a new quantity, named the union I , for triqubit pure states. The detailed formulation of the union I for a general triqubit pure state has

been given. Then we discussed the properties of the union I for different entanglements. Due to its convenient properties as a measure of entanglement, we introduced the total tangle $\tau^{(T)}$ that is equivalent to the union I from the mathematical point of view. An important advantage of the total tangle $\tau^{(T)}$ is that it can quantify the total entanglement of a triqubit pure state which neither the squared concurrence nor the 3-tangle can.

- Bounds to the union I in N -qubit pure states. Invoking an analogy to set theory, we gave a definition of the union I for an N -qubit pure state based on quantitative complementarity relations. This allowed us to prove operational necessary and sufficient separability criteria for N -qubit pure states, to formulate lower bounds to the union I for N -qubit pure states with different types of entanglement and to prove a sufficient condition for full entanglement.
- Detailed formulations of the union I for N -qubit pure states in conjecture. We generalized the entanglement Venn diagram to pure states of more than three qubits based on speculated quantitative complementarity relations. This allowed us to formulate the detailed forms of the union I for N -qubit pure states as a conjecture. The formulations of the total tangle $\tau^{(T)}$ for N -qubit pure states have been given by the corresponding union I .
- Multiparticle entanglement and ranks of density matrices. First, we discussed multiparticle pure-state entanglement by ranks of the reduced density matrices. Two necessary and sufficient conditions on entangled and fully entangled states have been proposed. Then we derived necessary conditions for the separability of multiparticle arbitrary-dimensional mixed states.

Following the results obtained in this thesis, there are many interesting problems for further research. Some of them are listed below:

- Detailed formulations of the union I for N -qubit pure states. We have obtained a detailed formulation of the union I for N -qubit pure states in this thesis, but the derivation of the union I is only based on speculated detailed quantitative complementarity relations. Thus validating the correctness of our results is necessary. One possibility of solving this problem is the search for exact definitions of measures for N -way entanglement which are unknown until now.

- Entanglement Venn diagrams and the union I for mixed states. In this thesis, we discussed the entanglement Venn diagram and the union I only in the case of pure states. Quantitative complementarity relations of mixed states have been discussed in [33, 34]. How to generalize our results about the entanglement Venn diagram and the union I to mixed states is an interesting and challenging problem for further research. We have made some attempts in this direction.
- Relations between two tools for studying entanglement: ranks of reduced density matrices and the positivity of the partial transpose. It is well known that the positivity of the partial transpose, introduced by Peres in 1996 [45], is a very important necessary condition for entanglement. Combinations of the rank and positive partial transpose criteria have been used to study the separability properties of some special composite systems [134–136]. It is an interesting problem for further research to investigate the relation between these two approaches in more detail.

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