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Quantification and Distribution of Genuinely Nonlocal Resources

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Zhaofeng Su

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Supervisor: Professor Yuan Feng

Centre for Quantum Software and Information

University of Technology Sydney

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CERTIFICATE OF ORIGINAL AUTHORSHIP

I certify that the work in this thesis has not previously been submitted for a degree nor has it been submitted as part of requirements for a degree except as fully acknowledged within the text.

I also certify that the thesis has been written by me. Any help that I have received in my research work and the preparation of the thesis itself has been acknowledged. In addition, I certify that all information sources and literature used are indicated in the thesis.

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TABLE OF CONTENTS

LIST OF FIGURES

ABSTRACT

Quantum mechanics is nonlocal, which makes it different from classical mechanics. Quantum information and quantum computation is a promising frontier science which is based on quantum mechanics. The nonlocality of quantum mechanics is the fundamental reason that many quantum information processing tasks have significant advantages over their classical counterparts.

In this dissertation, we study three aspects of quantum nonlocality, which include the quantitative relationship between entanglement and nonlocality, the quantification of genuine tripartite nonlocality and the distribution of nonlocal quantum resources. To be specific,

- We investigate the quantitative relationship between entanglement and nonlocality of bipartite quantum systems. We start by exploiting the condition that the nonlocality of two different two-qubit states can be optimally examined by a same nonlocality test setting. Via numerical simulation, we find that the nonlocality of a generic two-qubit state is upper bounded by a function of the corresponding entanglement. Further, we give an analytical proof for the upper bound and find the class of two-qubit states that can reach the upper bound.

- We analyze the quantification of genuine tripartite nonlocality of a generic three-qubit state. We find a method to solve the problem for a special class of three-qubit states which include not only pure states but also mixed states. Applying the method, we drive analytical results for the genuine tripartite nonlocality of generalized GHZ states, generalized Werner states and two class of mixed states with special correlation matrices.

- We investigate the distribution of nonlocal quantum resources. To distribute bipartite nonlocal quantum resources, we design an efficient quantum repeater scheme, which not only achieves the optimal transmission rate but also consumes less resources of local operations and classical communication, for the case of general pure states of two-qubit system. We also analyze the case of bipartite pure states of arbitrary dimensional quantum system and get an upper bound on the probability of a successful projection operation to produce a maximally nonlocal state. To distribute tripartite nonlocal resources, we propose a simple scenario to generate tripartite nonlocal resources from bipartite nonlocal resources. As examples, we examine the cases that two-qubit Werner states and general two-qubit pure states are prepared as resources, respectively. We get the upper bounds on the genuine tripartite nonlocality that can be generated in the scenario. We also provide the optimal measurement settings to achieve the upper bounds.

Keywords: Quantum mechanics; quantum information; local hidden variable model; CHSH inequality; Svetlichny inequality; genuine tripartite nonlocality.

1. INTRODUCTION AND BACKGROUNDS

Quantum mechanics and computer science are two of the most significant achievements of human being in the 20th century. Max Planck's contribution in 1900 led to the development of quantum mechanics. With the effort of a number of scientists for more than one century, quantum mechanics has fundamentally changed the human's view of the world and taught us to think the unthinkable. In 1965, Gordon Moore predicted the growth of computational power from the observation that the number of transistors in a dense integrated circuit doubles approximately every two years. This prediction is known as Moore's Law. In the last five decades, Moore's Law has been reliably predicted the pace of computer technology. The computational power of computers and the technology of communication not only continually speed up human's ability of understanding the nature but also make our everyday life more efficient and plenty.

Unfortunately, many scientists pointed out that Moore's Law would end in near future because that the classical computer technology is approaching its physical limitation. However, the continuous development of human being society has a thirst for faster and more powerful computers. Due to the indispensable significance of computational power, it is urgent to find a practical solution for improving the computational technology.

A possible solution to the failure of Moore's Law is to move to a new paradiagram which is based on the idea of using quantum mechanics to perform computational tasks, instead of classical physics. This paradiagram, which is a combination of quantum mechanical theory and computation theory, is known as quantum computation. The corresponding paradiagram for communication is known as quantum information.

Quantum computation and quantum information would have unimaginable advantages over their classical counterparts. Thus, the development of quantum computation and quantum information will probably cause a new technological revolution. The fundamental reason of those advantages is that quantum mechanics have the characteristics of entanglement and nonlocality.

1.1 Quantum computation and quantum information

As a potential substitution of classical computation technology, quantum computation is mainly motivated by two reasons. On one hand, there are many practical tasks that could not be solved by classical computers. One of the most important evidences is that there are essential difficulties in simulating quantum mechanical systems on classical computers. Due to this reason, the Nobel laureate Richard Feynman suggested that building computers based on the principles of quantum mechanics would allow us to void those difficulties [1].

On the other hand, physical theories give a limitation on the integration density of computer chips, which forecasts the failure of Moore's Law in near future [2, 3]. The major reason is that thermal fluctuations (Johnson-Nyquist noise) would case false bit. Another challenge is that the constrain of using lower supply voltages to keep power dissipation manageable contradicts with the requirement of increasing clock frequency. In recent years, industry practice also indicates that it becomes more and more difficult to follow Moore's Law [4, 5].

Feynman's proposition initiated the research field of quantum computation and quantum information. The potential failure of Moore's Law causes more attention of whole society on the research of the field. All of the world powers have put heavy investment on research programs related to quantum computation and quantum information. In the last three decades, remarkable progresses have been achieved in both theoretical and experimental aspects.

In classical computation, the Turing machine, which was invented in 1936 and named after its inventor, is a mathematical model of computation [6]. The Church-Turing thesis defined the mechanical computability of a Turing machine [7]. The Church-Turing principle indicates that every finitely realizable physical system can be perfectly simulated by a universal Turing machine operating by finite means. However, classical physics and the universal Turing machine do not obey the principle because that classical physics is continuous while the universal Turing machine is discrete [8]. Motivated by this drawback, a class of quantum Turing machines, the quantum analogues of Turing machines, have been proposed in the early 1980s [1, 9, 10]. In 1985, Deutsch defined a universal quantum Turing machine which is compatible with the Church-Turing principle [8]. The quantum Turing machine has many remarkable properties which are not reproducible by any classical Turing machine. It turns out that any function, which is computable in polynomial time by a quantum Turing machine, has a polynomial size quantum circuit [11]. This fact provides the theoretical possibility to construct a universal quantum computer. Not only the academia but also industry has great interest on realization of quantum computers. The first experimental quantum computer was demonstrated by Chuang *et al.* in 1998 [12]. Since the first demonstration of a 16-qubit quantum processor in 2007, the Canadian company D-Wave has updated its commercially available quantum computers for several rounds. In the early 2017, D-Wave released a quantum computer which is composed of 2000 qubits and has new control features [13]. The D-Wave quantum computers are specialized for the quantum annealing algorithm which is a method for finding the global minimum of a given function [14]. IBM scientists are aiming to build a universal quantum computer and recently released a 50-qubit quantum computer [15].

An algorithm is a sequence of step-by-step instructions for solving a practical problem. Algorithms are so important that they are known as the sprit of physical computers. The design of efficient quantum algorithms is the key for exploiting the magic power of quantum computers. Many clever quantum algorithms have been proposed in the last three decades. The first exponentially faster quantum algorithm is the Deutsch-Jozsa algorithm which was proposed by Deutsch and Jozsa in 1992 [16]. The most profound one is Shor's algorithm for factoring a large number in polynomial time [17]. RSA public-key cryptography scheme is difficult to be broken by a classical computer and widely used thereby. However, Shor's algorithm could be applied to break the RSA scheme. Shor's algorithm was firstly experimentally demonstrated in 2001 by factoring the number 15 on a nuclear magnetic resonance machine [18]. There are more significant quantum algorithms such as Grover algorithm for searching database [19], quantum walk algorithm for solving the element distinctness problem [20] and HHL algorithm for solving linear systems of equations [21]. All of them exhibit quadratic or even exponential quantum speedup over their best known classical counterparts.

In the last three decades, many significant quantum information processing protocols have been proposed. The first quantum key distribution protocol, proposed by Bennett and Brassard proposed in 1984, is usually referred as BB84 which is named after its inventors [22]. The BB84 protocol has been proved to be unconditional secure [23, 24]. In 1993, Bennett *et al.* designed a protocol to transmit quantum information via only local operations and classical communication (LOCC) and the help of the previously shared entanglement between the two ends [25]. This protocol achieves the transmission of unknown quantum information without directly sending a quantum system to the receiver, which is known as quantum teleportation. The speed of quantum teleportation is still limited by the speed of light because that classical communication is required in the process. Superdense coding is a quantum protocol to send two classical bits of information via transmitting only one qubit, which is somewhat like the inverse of quantum teleportation [26, 27]. The first experiment of quantum teleportation was realized by Bouwmeester *et al.* in 1997 [28]. In the August of 2016, Chinese scientists lunched a quantum science experiment satellite nicknamed Micius. According to the latest report, the distance of quantum teleportation was extended to 1400 km [29] and that of quantum key distribution was extended to 1200 km [30] by taking the ground-to-satellite diagram.

1.2 Quantum nonlocality

We have introduced quantum computation and quantum information which have greater advantage over their classical counterparts. One of the fundamental reasons of this advantage is that quantum mechanics has the characteristics of entanglement and nonlocality. In this section, we will give a brief introduction on quantum nonlocality.

In 1930s, physicists had concluded two basic principles for classical mechanics, namely locality and realism. The locality principle states that any property of an object is only determined by its immediate surroundings. In other words, the measurement outcome on one system would not be influenced by the measurement outcome of another remotely located system. The realism principle claims that any object must have a pre-existing value for any possible measurement before which is made. In 1935, Einstein, Podolsky and Rosen constructed a thought experiment to show that the theory of quantum mechanics contradicted with the theory of local realism. Therefore, they concluded that quantum mechanics was incomplete and should be supplemented with additional variables [31]. This thought experiment is also known as EPR paradox. Thereafter the EPR paper, Schrödinger pointed out that the phenomenon in EPR paradox was the characteristic of quantum mechanics and named it as *entanglement* [32].

In 1964, around 30 years after the publication of EPR paper, physicist John Stewart Bell from University of Wisconsin gave a negative answer to the EPR paradox [33]. Bell formulated the prediction of classical mechanics as a mathematical model which contains a hidden variable for restoring the theory of causality and locality. The model is also known as local hidden variable model (LHVM). Bell showed that the prediction based on quantum mechanics was impossible to coincide with that of LHVM, thereby concluding that quantum mechanics is nonlocal! Bell's groundbreaking work opens a new door for the research of quantum physics. In 1969, Clauser *et al.* proposed an inequality to certify the nonlocality of quantum mechanics in a simpler way [34]. Any prediction of LHVM satisfies the inequality while the prediction of quantum mechanics could violate it. Thus, the violation of the inequality by quantum predictions indicates that quantum mechanics is nonlocal. This inequality is known as CHSH inequality, named after its inventors. There are many inequalities which can confirm the nonlocality of quantum mechanics. Those inequalities are all known as Bell inequalities to commemorate the groundbreaking contribution of John Stewart Bell [35].

The predictions are usually expressed as conditional probability distributions which are also known as correlations. A correlation is local if it admits a LHVM. Otherwise, the correlation is nonlocal. The quantum state that can only generate local correlations is local state. If a quantum state can generate nonlocal correlation, then the state is said to be nonlocal quantum state. As nonlocal quantum states can generate correlations that cannot be created via classical experiments, they are a kind of precious resource for designing powerful protocols. Therefore, it is of practical significance to exploit the nonlocality of quantum states in both perspectives of qualitative verification and quantitative analysis.

It is difficult to verify the nonlocality of a quantum state via the LHVM. A clever way for the verification is through the violation of Bell-type inequalities which give upper bounds on all local quantum states. Thus, the violation of any Bell inequality is a sufficient condition for the state being nonlocal. Nonlocality of a correlation could be operationally measured by the tolerance of nonlocal correlations to the addition of noise[36, 37] or the amount of classical communication which has to be supplemented for reproducing the correlation from a local model [38]. A common choice for quantifying the nonlocality of a quantum state is through the amount of violation of a Bell inequality.

Recall that entanglement and nonlocality are the basic characteristics of quantum mechanics. The relationship between quantum entanglement and quantum nonlocality is a longstanding problem in the quantum foundation research. In the earlier years since Bell's proposal of nonlocality, entanglement and nonlocality were thought to be the same concept. Indeed, all entangled pure states are also nonlocal states [39]. However, this result is not true for mixed states. In 1989, Werner found a class of quantum states which are entangled but admits some LHVM [40]. Those quantum states are known as Werner states. The presence of Werner states indicates that being entangled is not a sufficient condition to be nonlocal. By quantitatively analyzing the nonlocality of general two-qubit pure states, Brunner *et al.* concluded that entanglement and nonlocality are different resources [41]. It is shown that all quantum states which are useful for quantum teleportation are nonlocal resources [42] while not all entangled states are useful for teleportation [43].

The simplest nonlocality test scenario is the one with two parties each of whom has two possible dichotomic measurement settings. CHSH inequality is the only nontrivial Bell inequality for the bipartite nonlocality test scenario [44]. The nonlocality of this scenario has been extensively studied in the last five decades. In 1995, Horodecki *et al.* found a necessary and sufficient condition for violating the CHSH inequality [45]. They got an analytical expression for the maximal violation of the CHSH inequality by an arbitrary two-qubit state. The violation of CHSH inequality was firstly demonstrated in physical experiment by Freedman and Clauser in 1972 [46]. In recent years, many research groups have been concentrating on the loophole free test of Bell's theorem [47, 48, 49, 50].

The nonlocality of multipartite scenario has a much more complex structure than the case of bipartite scenario, which makes the research of multipartite nonlocality an interesting but challenging work. The simplest multipartite nonlocality test scenario is the one with three participants. Different notations of tripartite nonlocality can be defined based on the nonsignaling constraint between participants or the order of test measurements [51]. The genuine tripartite nonlocality, a more precious nonlocal resource, is based on a LHVM proposed by Svetlichny in 1987 [52]. Svetlichny also constructed a Bell inequality, known as Svetlichny inequality, to detect the genuine tripartite nonlocality. Svetlichny's tripartite genuine nonlocality model has been generalized to n parties and the corresponding Bell-type inequality has been derived [53, 54]. We will focus on Svetlichny's definition in this dissertation.

Due to the complex structure, the genuine tripartite nonlocality has not been fully understood, even for the three-qubit system. In the simplest nonlocality test scenario, a three-qubit quantum system is shared by the participants in the scenario and each participant performs a dichotomic measurement chosen from two possible measurement settings. The genuine tripartite nonlocality of the three-qubit system can be quantified by the maximal Svetlichny inequality violation of the state. A comprehensive measure can be further constructed from the maximal violation. Note that the Svetlichny inequality gives an upper bound 4 for any local correlation that admits a tripartite LHVM. However, the inequality can be violated when quantum resource is shared in the scenario. The maximal violation of the inequality is $4\sqrt{2}$, which can be achieved by the GHZ state.

It is difficult to analytically analyze the genuine nonlocality of a general three-qubit state. Progress was achieved in 2009 when Ghose *et al.* derived an analytical expression of genuine nonlocality for the generalized GHZ states and W states [55]. They also found the quantitative relationship between the entanglement and nonlocality of the states. Later in 2010, Ajoy and Rungta [56] extended this result to a set of more general GHZ-class states and W-class states. The genuine nonlocality of three-mode Gaussian states of continuous variable systems was investigated by Adesso and Piano in 2014 [57]. In 2016, Paul *et al.* investigated different notions of nonlocality of the three-qubit GHZ-symmetric states [58]. Recently, a tight upper bound for the genuine nonlocality of general three-qubit states was obtained by Li *et al.* [59]. In experiment, three-photon GHZ states are generated to test the genuine tripartite nonlocality through the violation of the Svetlichny inequality [60, 61].

The quantitative relationship between entanglement and nonlocality of a three-qubit system is an interesting problem. However, few progresses have been achieved on this problem because of the difficulty of quantifying tripartite nonlocality. Numerical analysis shows that there are upper and lower bounds on entanglement for a three-qubit state with given nonlocality [62]. The analytical relationship for a special class of three-qubit pure state were found [55, 56]. It is still an open problem to find an analytical relationship for general two-qubit states.

Interestingly, nonlocality could be super-activated from local resources. In 1995, Popescu firstly noticed that a class of quantum states are classical when single measurement is considered while they present non-classical feature when each system is subjected to a sequence of ideal measurements [63]. This type of nonlocality is known as hidden nonlocality. Further, it also shows that bipartite nonlocality can be enhanced by collective measurements [64]. More surprisingly, quantum nonlocality can be super-activated from classical resources in a quantum network [65].

Despite LHVM, nonlocality can also be operationally interpreted. Inspired by the operational definition of quantum entanglement, Gallego *et al.* concluded that nonlocality is a resource that could not be created by the operation of wirings and classical communications prior to the inputs [66]. They also systematically studied the nonlocality generated by the sequential quantum measurements, which is known as the time ordered framework of quantum nonlocality [67]. The operational definition of quantum nonlocality turns out to be equivalent to the time ordered framework of nonlocality. Those interpretations of quantum nonlocality enrich our understanding of quantum mechanics.

1.3 Motivations and contributions

In the previous sections, we have seen that quantum nonlocality not only plays an indispensable role in the application of quantum processing tasks but also has the fundamental importance in the theory of quantum mechanics. However, there are important issues to be resolved both in fundamental theories and practical applications.

In particular, there are problems not well understood with respect to quantum entanglement and nonlocality. Such as the relationship between nonlocality and entanglement of a quantum system, the quantification of the genuine nonlocality in a tripartite quantum system and the distribution of nonlocal quantum resources.

We consider three problems in this dissertation. The first concern is the relationship between the nonlocality and the entanglement of a general two-qubit state. The qualitative relationship have been extensively studied in literatures. The quantitative relationship of the class of two-qubit pure states is also simple to verify. However, the quantitative relationship between the nonlocality and entanglement of a general two-qubit state is unclear. This led to the question listed as follows:

Question 1. *Can we quantitatively drive a more close relationship between the nonlocality and entanglement of a general two-qubit state?*

Our second concern is the quantification of the genuine tripartite nonlocality of a general three-qubit state, which is a complex and long standing problem. According to the aforementioned references, analytical results of this problem have been only examined for a few of very simple three-qubit states. Thus, it naturally leads to the following question.

Question 2. *Can we find a method for quantitatively analyzing the genuine tripartite nonlocality of a general three-qubit state?*

The last concern is the distribution of nonlocal quantum resources. The nonlocal quantum resources are indispensable for many important quantum information processing tasks. In most quantum information applications, the nonlocal quantum resources should be distributed in a network which consists of many separated participants. Note that nonlocality is a type of resource that could not be created via LOCC. Namely, quantum nonlocal resource is originally created at a same place and then sent to different participants.

However, in experimental practice, it is difficult to transmit quantum resources over long distance. There is a trade-off between the distance and the rate of the transmission of quantum states. A practical solution to this problem is the scheme of quantum repeaters which extend the distance of quantum resource distribution with acceptable transmission rate. In the aforementioned references of quantum repeaters, LOCC is considered as an unlimited resource. Thus, we propose a question listed as follows:

Question 3. *Utilizing the basic scheme of quantum repeaters, can we design a more effective protocol to distribute nonlocal quantum resources?*

In this dissertation, we exploit the questions described above. The main contributions of this dissertation are summarised as follows:

1. For Question 1, we find out that the nonlocality of a general two-qubit state is upper bounded by a function of the corresponding entanglement. Further, we figure out the class of two-qubit states that can achieve the upper bound. As a prerequisite question, we also exploit the possibility of testing the nonlocality of different two-qubit states by the same nonlocality test setting. We give the condition that two different general two-qubit states could have the same optimal nonlocality test setting. We prove that at most two different two-qubit pure states can share the same optimal nonlocality test setting. Moreover, we find out the class of such two-qubit pairs.
   Related publication:
   - Zhaofeng Su and Lvzhou Li. The nonlocality of two-qubit system is upper bounded by the entanglement. (Pending submission)

2. For Question 2, we find a more practical method to quantitatively analyze the genuine tripartite nonlocality of a general three-qubit states. Applying the method, we can get the analytical results for a class of special three-qubit states. The method applies not only for all three-qubit states which have been analyzed in literatures, but also for a more general class of three-qubit states. The class of three-qubit states include generalized GHZ states, generalized Werner states and two classes of mixed states with special correlation matrices.
   Related publication:
   - Zhaofeng Su, Lvzhou Li, and Jie Ling. An approach for quantitatively analyzing the genuine tripartite nonlocality of general three-qubit states.

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3. For Question 3, we design effective protocols for the distribution of both bipartite and tripartite nonlocal quantum resources.

   To distribute bipartite quantum resources, we present some effective quantum repeaters with respects to both transmission rate of quantum resources and LOCC complexity. We construct a protocol to distribute two-qubit maximally entangled states at optimal transmission rate with less LOCC complexity. We also analyze the distribution of a general bipartite pure state and get the upper bound on the probability of a successful projection to produce a maximally entangled state.

   To distribute tripartite quantum resources, we propose a simple scenario to generate genuinely tripartite nonlocal state from bipartite nonlocal states. We analyze the resources of general pure states and Werner states of a two-qubit system. We get the upper bounds on the genuine tripartite nonlocality that can be generated in the scenario and provide the optimal measurement settings to achieve the upper bound.

   Related publications:

   - Zhaofeng Su, Ji Guan, and Lvzhou Li, Efficient quantum repeater in perspective of both entanglement concentration rate and LOCC complexity, *Physical Review A*, 97:012325, January 2018. DOI: 10.1103/PhysRevA.97.012325
   - Zhaofeng Su. Generating tripartite nonlocality from bipartite resources. *Quantum Information Processing*, 16: 28, January 2017. DOI:10.1007/s11128-016-1493-7

1.4 Outline of the thesis

The remainder of the dissertation is organized as follows:

1. Chapter 2 introduces the preliminaries of the dissertation which include the mathematical tools, the fundamental theory of quantum mechanics, the ba-

sic ideas of quantum information and the technical introduction of bipartite nonlocality.

2. Chapter 3 firstly reviews the measures of entanglement and nonlocality of a two-qubit system. Then, we discuss the problem of optimally testing the nonlocality of different two-qubit states by the same measurement setting. Finally, we get a quantitative relationship between the nonlocality and the entanglement of a two-qubit state.

3. Chapter 4 discusses the quantification of genuine tripartite nonlocality of the general three-qubit states. As the first step, we introduce the definition and verification of genuine tripartite nonlocality. Then, we quantitatively analyze the genuine tripartite nonlocality of a general three-qubit state. We propose a strategy for quantifying the genuine tripartite nonlocality and find several properties to simplify the problem. At last, we apply the strategy and properties to derive analytical results of the genuine tripartite nonlocality for four important classes of three-qubit states.

4. Chapter 5 discusses the distribution of nonlocal quantum resources. We analyze the challenges and possible solutions of the problem. We propose an effective quantum repeater scheme for distributing two-qubit nonlocal resources, which not only achieves the optimal transmission rate but also consumes less resources of LOCC. We also propose a scenario for distributing tripartite nonlocal resources which is realized by generating tripartite nonlocality from bipartite nonlocal resources. We analyze the cases of preparing two-qubit Werner states and general two-qubit pure states as resources.

5. Chapter 6 concludes the dissertation and proposes the problems for future research.

2. PRELIMINARIES

Nonlocality is a unique characteristic of quantum mechanics, which makes quantum computation and quantum information have great advantages over their classical counterparts. To have a better understand and further research on quantum nonlocality and its applications, it is necessary to know some preliminaries about the related subjects. This chapter contains the necessary preliminary knowledge for understanding the dissertation.

In Section 2.1, we give a brief introduction on linear algebra which is the mathematical foundation for the theory of quantum mechanics and the theory of quantum computation and information. Then, we introduce the fundamental theory of quantum mechanics in Section 2.2 and the preliminary knowledge of quantum information in Section 2.3. Finally, we technically explicate the theory of nonlocality by introducing the bipartite nonlocality in Section 2.4. Most of the preliminaries can be found in the book *Quantum Computation and Quantum Information* [68], which is regarded as a standard text on the subject.

2.1 Linear algebra

Linear algebra is a discipline that deals with vectors, vector spaces and operators. Quantum mechanics is highly inspired by the notations of linear algebra. Thus, linear algebra also acts as a fundamental mathematics tool for describing quantum mechanics. Dirac notation, named after its inventor, is very useful in quantum mechanics. We will inherit this notation for the description of linear algebra and quantum information.

Any vector space, denoted by V, is associated with a field F. The elements of the vector space are vectors while the elements of the field are known as scalars. In quantum mechanics, the field is usually the field of complex numbers. Thus, the field considered in this dissertation is the complex field if no further specification is given. A vector space is equipped with two operations, namely vector addition and scalar multiplication. A vector in V is denoted by a *ket* $|\psi\rangle$ where the notation $|\cdot\rangle$ indicates that the object is a vector and ψ is the label of the vector. A vector space is closed under the two operations. That is, $a|\psi\rangle + b|\phi\rangle$ is an element of V for any vectors $|\psi\rangle, |\phi\rangle \in V$ and scalars $a, b \in F$.

A set of vectors $\{|\psi_1\rangle, |\psi_2\rangle, \cdots, |\psi_n\rangle\}$ is called a spanning set of the space V if any vector $|\psi\rangle$ in the space can be written as a linear combination $|\psi\rangle = \sum_{k=1}^{n} a_k|\psi_k\rangle$ of the vectors in the set where $a_k \in F$ for all k ranging from 1 to n. We also say that the space V is spanned by the spanning set. If n is the minimum number such that the set is a spanning set for the space V, we say that the set of vectors is a basis of the space and the number n is the space's dimension.

Suppose V and W are two vector spaces over the same filed F. A linear operator A between V and W is defined as a function $A : V \to W$ which takes any vector $|v\rangle$ in V to the corresponding vector $A(|v\rangle)$ in W. The function is linearly in its inputs,

$$A(\sum_j a_j|v_j\rangle) = \sum_j a_j A(|v_j\rangle). \tag{2.1}$$

We usually denote the function $A(|v\rangle)$ as $A|v\rangle$. When W is the same vector space as V , we say that A is a linear operator defined on the vector space V. Identity operator I and zero operator 0 are two special linear operators on a vector space. Any input vector in the vector space is invariant under the identity operator and is transformed to zero vector by the zero operator.

An inner product of the vector space V is a function $(|v\rangle, |w\rangle)$ which maps two vectors $|v\rangle$ and $|w\rangle$ of V to a complex number. The inner product function is required to be conjugate symmetric and linear in the second argument. It is also required that $(|v\rangle, |v\rangle) \geq 0$ with equality if and only if $|v\rangle = 0$. The standard quantum mechanical notation for the inner product is $\langle v|w\rangle$ where $\langle v|$ is the dual vector to $|v\rangle$. The dual vector $\langle v|$ is also known as a *bra*. The bra-ket notation was introduced by Pual Dirac in 1939 for describing quantum states [69] which are standard notations in modern quantum mechanics. A vector space with inner product is known as Hilbert space which is an indispensable tool in the theory of quantum mechanics. We usually denote a Hilbert space of dimension n as $\mathcal{H}_n$. Tow vectors are said to be orthogonal if their inner product is equal to 0. A norm is a function that signs a strictly positive length to each vector in the space. Based on the definition of inner product, we can define the norm of a vector $|v\rangle$ as $\||v\rangle\| \equiv \sqrt{\langle v|v\rangle}$. A vector with norm being 1 is called unit vector. A set of vectors is said to be an orthonormal set if all vectors in the set are unit vectors and they are orthogonal to each other. If a basis of a vector space is an orthonormal set, we say that the set is an orthonormal basis of the vector space.

The concepts we have introduced are consistent with the matrix notations for linear algebra. Suppose $\{|\psi_1\rangle, \cdots, |\psi_n\rangle\}$ and $\{|\phi_1\rangle, \cdots, |\phi_m\rangle\}$ are orthonormal basis for the vector spaces V and W, respectively. Any vector $|v\rangle$ in V can be written as $|v\rangle = \sum_{k=1}^{n} v_k |\psi_k\rangle$. We can think the ket $|v\rangle$ as a column vector. The coefficients $v_1, \cdots, v_n$ can be viewed as the column elements of $|v\rangle$ under the basis $\{|\psi_1\rangle, \cdots, |\psi_n\rangle\}$. The corresponding bra $\langle v|$ can be defined as a row vector $\langle v| \equiv [v_1^*, \cdots, v_n^*]$ which is the conjugate transpose of the column vector of $|v\rangle$. The similar consistences apply for the vector space W. Suppose A is a linear operator from V to W. As $A|\psi_i\rangle$ is a vector in W, there is a unique collection of numbers a_{ji} with $i = 1, \cdots, n$ and $j = 1, \cdots, m$ such that $A|\psi_i\rangle = \sum_{j=1}^{m} a_{ji}|\phi_j\rangle$. The behavior of A is completely described by the collection of numbers a_{ji}. Thus, we can also think A as a $m \times n$ matrix with elements a_{ji}. We will interchangeably use the notation A for operator and matrix. Suppose $|v'\rangle = \sum_{k=1}^{n} v'_k |\psi_k\rangle$ is an arbitrary vector in V. An inner product of the space V can be defined as

$$\langle v|v'\rangle = \sum_{k=1}^{n} v_k^* v'_k, \tag{2.2}$$

which is equal to the matrix production of the corresponding row vector and column vector. A norm of the vector $|v\rangle$ is $\||v\rangle\| = \sum_{k=1}^{n} |v_k|^2$.

Suppose A is any linear operator on a Hilbert space V. An eigenvector of A is a nonzero vector $|\alpha\rangle$ such that $A|\alpha\rangle = \lambda|\alpha\rangle$ where λ is a scalar known as the eigenvalue of A corresponding to the eigenvector $|\alpha\rangle$. A popular way to find out the eigenvalues of A is to solve the characteristic equation $\det|A - \lambda I| = 0$. The adjoint of A, denoted as $A^\dagger$, is a unique linear operator such that $(|v\rangle, A|v'\rangle) = (A^\dagger|v\rangle, |v'\rangle)$ for all vectors $|v\rangle, |v'\rangle \in V$. The matrix representation of $A^\dagger$ is the conjugate transpose of A's matrix representation, namely, $A^\dagger = (A^*)^T$. There are classes of special linear operators. Those that are frequently used in quantum mechanics and quantum computation are introduced as follows:

- **Hermitian operator**. A is called a Hermitian operator if $A^\dagger = A$.

- **Normal operator**. A is called a normal operator if $A^\dagger A = AA^\dagger$.

- **Unitary operator**. A is called a unitary operator if $A^\dagger A = AA^\dagger = I$.

- **Positive operator**. A is called a positive operator if $\langle v|A|v\rangle \geq 0$ for any vector $|v\rangle \in V$.

- **Projector**. Suppose W is a subspace of V. $\{|w_1\rangle, \cdots, |w_m\rangle\}$ is an orthonormal basis of W. Let $P \equiv \sum_{k=1}^{m} |w_k\rangle\langle w_k|$. Then, we say that P is a projector onto the vector space W.

It turns out that any positive operator is also a Hermitian operator. Both Hermitian operators and unitary operators are normal operators. Any normal operator A on the vector space V has a spectral decomposition of the form as

$$A = \sum_k \lambda_k |\varphi_k\rangle\langle\varphi_k|, \tag{2.3}$$

where every λ_k is the eigenvalue of the operator A and $|\varphi_k\rangle$ is the eigenvector of A with the eigenvalue λ_k. The set of eigenvectors $\{|\varphi_k\rangle\}$ forms an orthonormal basis for the space V.

Trace is an operation which maps a linear operator on a vector space to a complex number. The trace of an operator A on the vector space V is defined as

$$tr(A) = \sum_k \langle\psi_k|A|\psi_k\rangle, \tag{2.4}$$

where $\{|\psi_k\rangle\}$ is an orthonormal basis for the space V. The trace of an operator is invariant to the orthonormal basis chosen for the corresponding vector space. Suppose B is another linear operator on V, $|\psi\rangle$ is an arbitrary vector in V and z is a complex number. It is obvious that the trace operation has some properties listed as follows:

- $tr(A + B) = tr(A) + tr(B)$,

- $tr(AB) = tr(BA)$,

- $tr(zA) = ztr(A)$,

- $tr(A|\psi\rangle\langle\psi|) = \langle\psi|A|\psi\rangle$.

Considering in perspective of matrix representation, $tr(A)$ is equal to the sum of the diagonal elements of matrix A.

Pauli matrices is a set of three 2×2 complex matrices. Together with the identity matrix, Pauli matrices play an important role in quantum mechanics and quantum information. They are defined as follows:

$$\sigma_0 \equiv I \equiv \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \qquad \sigma_1 \equiv \sigma_x \equiv X \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$
$$\sigma_2 \equiv \sigma_y \equiv Y \equiv \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \qquad \sigma_3 \equiv \sigma_z \equiv Z \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Note that Pauli matrices are Hermitian and unitary. They form a basis for the vector space of 2×2 Hermitian matrices with real coefficients. Any 2×2 Hermitian matrix H can be written as $H = \sum_{k=0}^{3} r_k \sigma_k$ where $r_k \in \mathbb{R}$ for all $k = 0, 1, 2$ and 3. Pauli matrices also form a basis for the space of all 2×2 matrices with complex coefficients.

Tensor product, denoted by $\otimes$, is a method for generating a larger vector space by associating two small vector spaces together. Taking the assumptions we have made, V and W are two vector spaces over complex field with the orthonormal basis $\{|\psi_1\rangle, \cdots, |\psi_n\rangle\}$ and $\{|\phi_1\rangle, \cdots, |\phi_m\rangle|\}$, respectively. Then, $V \otimes W$ is a vector space of dimension $m * n$. For any vectors $|v\rangle \in V$ and $|w\rangle \in W$, their tensor product $|v\rangle \otimes |w\rangle$, usually denoted as $|v\rangle|w\rangle$ or $|v, w\rangle$, is an element of the vector space $V \otimes W$. An orthonormal basis for the vector space $V \otimes W$ is $\{|\psi_j\rangle \otimes |\phi_k\rangle | j = 1, \cdots, n \text{ and } k = 1, \cdots m\}$.

2.2 The basic theory of quantum mechanics

Due to the special role of quantum mechanics in nonlocality and quantum information, it is necessary to understand the basic theory of quantum mechanics. However, quantum mechanics is one of the most difficult subjects for those who do not have any background on physics. This is because that quantum mechanics is always introduced in the perspective of wave functions in traditional course. Fortunately, scientists have concluded quantum mechanics with four postulates which are easily grappled by the non-expert. The postulates act as an interface between the theory of quantum mechanics and the research of quantum computation and quantum information. Benefitted from such an interface, more and more researchers with the background of computer science get involved in the research work of quantum computation and quantum information. In this section, we will introduce the postulates of quantum mechanics.

Postulate 1 (Quantum state space)**.** *Any isolated quantum system is associated with a Hilbert space which is known as the state space of the system. The system is completely described by a unit vector, which is known as the state vector of the system, in the system's state space.*

This postulate defines the mathematical arena where quantum mechanics takes place. The following postulates describe how a quantum system evolves over time and what it will happen when we measure it.

Postulate 2 (Quantum evolution)**.** *The evolution of a closed quantum system is described by a unitary operator. Suppose the state of the system at time t_1 is $|\psi\rangle$ and it becomes $|\psi'\rangle$ at time t_2. Then, the states of the system at different times is related by a unitary U which only depends on the times t_1 and t_2 such that*

$$|\psi'\rangle = U|\psi\rangle. \tag{2.5}$$

Postulate 3 (Quantum measurement)**.** *Any quantum measurement is described by a collection $\{M_m\}$ of measurement operators which satisfy the completeness relation $\sum_m M_m^\dagger M_m = I$. Those operators act on the state space of the quantum system. Each index m corresponds to a measurement outcome which may occur in the quantum measurement experiment. Suppose the system is in the state $|\psi\rangle$ immediately before the measurement. Then, the probability of observing the result m is*

$$p(m) = \langle\psi|M_m^\dagger M_m|\psi\rangle. \tag{2.6}$$

If we have observed the outcome m, the system would be in the state

$$|\psi_m\rangle = \frac{M_m|\psi\rangle}{\sqrt{p(m)}}. \tag{2.7}$$

The measurement defined in Postulate 3 is known as general quantum measurement. A special quantum measurement is projective measurement which is known as von Neumann measurement.

(Projective measurement) A projective measurement on a quantum system is described by a Hermitian operator M, which is known as an observable, on the state space. The observable has a spectral decomposition of the form $M = \sum_m mP_m$ where P_m is the projector onto the eigenspace of M with eigenvalue m. Every eigenvalue m corresponds to a possible measurement outcome. Measuring the state $|\psi\rangle$ with the observable M, the probability of observing result m is

$$p(m) = \langle\psi|P_m|\psi\rangle. \tag{2.8}$$

On condition that the result m is observed, the state of the system after the measurement is

$$|\psi_m\rangle = \frac{P_m|\psi\rangle}{\sqrt{p(m)}}. \tag{2.9}$$

Projective measurements are frequently concerned in many applications of quantum computation and quantum information. It turns out that any general measurement is equivalent to a projective measurement with assistance of unitary transformations.

The basic quantum system is the one corresponding to the Hilbert space of dimension 2. Any observable with eigenvalues $+1$ and -1 of the basic system can be represented by a three dimensional real unit vector $\vec{r} = (r_1, r_2, r_3)$. The corresponding observable reads

$$\vec{r}\cdot\vec{\sigma} \equiv r_1\sigma_1 + r_2\sigma_2 + r_3\sigma_3. \tag{2.10}$$

The projectors corresponding to eigenvalues $+1$ and -1 of the observable $\vec{r}\cdot\vec{\sigma}$ are $P_+ = \frac{1}{2}(I + \vec{r}\cdot\vec{\sigma})$ and $P_- = \frac{1}{2}(I - \vec{r}\cdot\vec{\sigma})$, respectively.

Postulate 4 (Composite systems)**.** *A composite quantum system can be built-up by bringing a collection of independent quantum systems. The state space of the composite system is the tensor product of the state space of the individual systems. The composite system can be described by a unit vector in the state space.*

The above postulate tells us that serval individual quantum systems can be viewed as a larger quantum system. Suppose a collection of quantum systems $H_1, \cdots, H_t$ are in the states $|\psi_1\rangle, \cdots, |\psi_t\rangle$, respectively. Then, the composite system $H_1 \otimes \cdots \otimes H_t$ is in the state $|\psi_1\rangle \otimes \cdots \otimes |\psi_t\rangle$.

The quantum states introduced in the above postulates are pure states. Mathematically, they are represented by unit vectors in Hilbert spaces. In fact, there are quantum systems that cannot be described by pure states. Namely, they are in mixed states. Mixed states can be interpreted in perspective of a probabilistic quantum source. Suppose we have a black box in which there are n quantum devices which can emit quantum states $|\psi_1\rangle, \cdots, |\psi_n\rangle$ with probability $p_1, \cdots, p_n$, respectively. When the black box emits a quantum system, we only know the state of the system probabilistically. Thus, we say that the system is in a mixed state. Such a mixed state can be described by an operator defined as

$$\rho = \sum_{k=1}^{n} p_k |\psi_k\rangle\langle\psi_k|. \tag{2.11}$$

The operator ρ of the above form is known as a density operator. The statistics $\{p_k, |\psi_k\rangle\}$ of the system is called an ensemble of pure states. Note that any mixture of quantum states is again a valid quantum state. Any quantum state that cannot be written as a mixture of other states is a pure state. Otherwise, it is a mixed state.

Any density operator is a positive operator with trace 1. The converse is also true. The purity of a quantum state ρ is defined as $tr(\rho^2)$ [70]. The value of $tr(\rho^2)$ ranges from $\frac{1}{d}$ to 1 where d is the dimension of the system's state space. The state ρ is a pure state if and only if the purity $tr(\rho^2) = 1$. The lower bound is obtained by the maximally mixed state, represented by $\frac{I_d}{d}$. A density operator may correspond to different ensembles. Two different ensembles $\{p_k, |\psi_k\rangle\}$ and $\{q_j, |\phi_k\rangle\}$ give rise to a same density operator if and only there is a unitary matrix with elements u_{kj} such that $\sqrt{p_k}|\psi_k\rangle = \sum_j u_{kj}\sqrt{q_j}|\phi_k\rangle$.

The density operator language is a more general description for quantum systems. Any quantum system in a pure state can be described by a density operator. In the following, we reformulate the postulates of quantum mechanics in terms of the density operator language.

Postulate 1$'$. *Associated to any isolated quantum system is a Hilbert space which is known the state space of the system. The system is completely described by a density operator acting on the state space.*

Postulate 2$'$. *The evolution of a closed quantum system is described by a unitary transformation . Suppose the system is in the states ρ and ρ' at time t and t', respectively. Then, the states of the system is related by a unitary operator U on the state space in the form as follows*

$$\rho' = U^\dagger \rho U. \tag{2.12}$$

Postulate 3$'$. *The experimental measurement of a quantum system can be described by a collection $\{M_m\}$ of measurement operators which act on the state space of the quantum system and satisfy the completeness relation $\sum_m M_m^\dagger M_m = I$. Each index m of the measurement operators corresponds to a possible measurement outcome which may be observed in the quantum measurement experiment. Suppose the system is in the state ρ immediately before the measurement. Then, the probability of observing outcome m is*

$$p(m) = tr(M_m^\dagger M_m \rho), \tag{2.13}$$

and the state of the system after observing m is

$$\rho_m = \frac{M_m \rho M_m^\dagger}{\sqrt{p(m)}}. \tag{2.14}$$

Postulate 4$'$. *A composite quantum system can be built-up by bringing a collection of independent quantum systems. The state space of the composite system is the tensor product of the state space of the individual systems. The composite system can be described by a density operator on the state space.*

The Postulate 4$'$ can interpret the fact that any global phase of a pure does not make sense. Namely, the state $e^{i\varphi}|\psi\rangle$ has the same experimental statistics with the state $|\psi\rangle$. One should note that the two pure states correspond to a same density operator.

2.3 Foundations of quantum information theory

Quantum nonlocality and quantum entanglement are indispensable resources for quantum computation and quantum information, which makes the research of nonlocality have excess practical significance. In this section, we will give a brief introduction on the preliminary of quantum information.

2.3.1 Quantum bit and Bloch sphere

In classical computer science, the basic unit of information is called a bit which takes value 0 or 1. In quantum computation and quantum information, the basic unit of information is a quantum bit which is abbreviated as *qubit*. Utilizing the notations of quantum mechanics, the state of a qubit is represented by Dirac notation $|\cdot\rangle$. A qubit not only can be in the state $|0\rangle$ or $|1\rangle$, but also can be in a superposition represented as

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \tag{2.15}$$

where α and β are complex numbers with the unit constraint $|\alpha|^2 + |\beta|^2 = 1$.

The physical object of a qubit is a quantum system of which the state space is of dimension 2. The states $|0\rangle$ and $|1\rangle$ forms an orthonormal basis of the state space. Thus, the state shown in Eq. (2.15) is the general pure state of a qubit system. Up to some ignorable global phase, the state of a general qubit system can be equivalently written as

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle, \tag{2.16}$$

where $\theta \in [0, 2\pi]$ and $\varphi \in [0, 2\pi)$.

It is interesting that any pure state corresponds to a point on the unit three-dimensional sphere which is known as Bloch sphere. The Bloch sphere provide a geometrical representation of the state of a single qubit. Many properties and operations on single qubits can be conveniently described with the Bloch sphere. The general pure state $|\psi\rangle$ can be visualized on the Bloch sphere showen in the Figure 2.1. The coordinate corresponding to the state $|\psi\rangle$ is $(1, \theta, \varphi)$ in perspective of spherical coordinate system while that is $(sin\theta\cos\varphi, sin\theta\sin\varphi, \cos\theta)$ in perspective of Cartesian coordinate system.

A qubit system could also be in a mixed state. Any mixed state ρ of a qubit can be represented by a three-dimensional real vector $\vec{r} = (r_1, r_2, r_3)$ with norm $\|\vec{r}\| \leq 1$ such that

$$\rho = \frac{1}{2}(I + \vec{r}\cdot\vec{\sigma}), \tag{2.17}$$

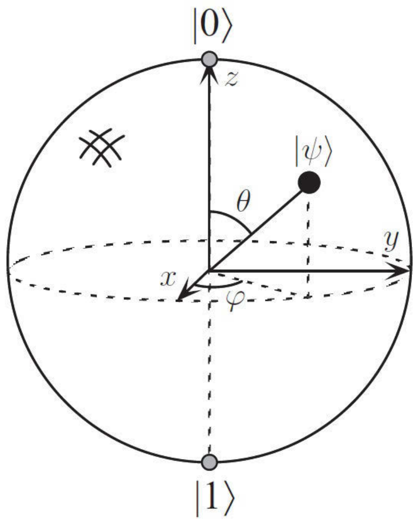

Fig. 2.1: Bloch sphere representation of a qubit.

where $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is the vector of Pauli matrices. The elements of $\vec{r}$ can be obtained through the relation $r_k = tr(\sigma_k \rho)$ for $k = 1, 2, 3$. Thus, any mixed state of a single qubit can be visualized as a point insider the Bloch sphere. $\|\vec{r}\| = 1$, which indicates the point is on the surface of the Bloch sphere, if and only if when ρ is a pure state.

Analogous with the classical computer science, there are gates in quantum computation for the manipulations of information. Mathematically, any quantum gate is represented by a unitary matrix on the corresponding state space. The quantum gates on a single qubit are 2×2 unitary matrices. All Pauli matrices represent important quantum gates. We need to point out that the gate represented by Pauli matrix X is known as quantum NOT gate. Another important quantum gate is Hadamard gate, represented by $H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$. The Hadamard gate transform the states $|0\rangle$ and $|1\rangle$ to $|+\rangle \equiv (|0\rangle + |1\rangle)/\sqrt{2}$ and $|-\rangle \equiv (|0\rangle - |1\rangle)/\sqrt{2}$, respectively. $\{|+\rangle, |-\rangle\}$ also acts as an orthonormal basis of the state space of a qubit system.

Geometrically, unitary transformation on a single qubit system corresponds to a rotation of the system's state vector on the Bloch sphere. Any unitary U on $\mathcal{H}_2$ can written as $U = e^{i\alpha} R_{\vec{n}}(\theta)$ where $R_{\vec{n}}(\theta) \equiv \cos\frac{\theta}{2} I - i \sin\frac{\theta}{2}(\vec{n} \cdot \vec{\sigma})$ is a rotation by θ about the $\vec{n}$ axis where $\vec{n}$ is a unit vector in $\mathbb{R}^3$. Suppose the spectral decomposition of U is $U = e^{i\theta_1}|\psi_1\rangle\langle\psi_1| + e^{i\theta_2}|\psi_2\rangle\langle\psi_2|$. Then, the axis $\vec{n}$ is the vector representation of the pure state $|\psi_1\rangle$ on the Bloch sphere. The rotation angle is $\theta = \theta_2 - \theta_1$ and the phase of the unitary is $\alpha = \theta_1 + \theta_2$.

2.3.2 Quantum register of multiple qubits

In classical computer science, the term register stands for a physical device where some finite data can be stored and manipulated. Any compound of registers is also a register. The quantum analog of the classical register is quantum register where quantum information may be stored and manipulated. A quantum register is a system comprising multiple qubits [71].

The most basic register of multiple qubits is the one that contains two qubits. Any density operator ρ on the state space of the basic register can be equivalently written as

$$\rho = \frac{1}{4}(I \otimes I + \vec{r} \cdot \vec{\sigma} \otimes I + I \otimes \vec{s} \cdot \vec{\sigma} + \sum_{j,k=1}^{3} t_{jk}\sigma_j \otimes \sigma_k), \tag{2.18}$$

where $\vec{r}$ and $\vec{s}$ are vectors in $\mathbb{R}^3$ with norm no greater than one and $t_{jk} = tr(\sigma_j \otimes \sigma_k \rho)$ are real numbers.

An important quantum gate on two-qubit systems is the controlled-NOT, which is often referred as CNOT. The CNOT gate has two input qubits where the first input qubit is known as control qubit while the second one is known as target qubit. The target qubit will be flipped only when the control qubit is activated. Mathematically, the CNOT gate can be represented written as $CNOT = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes X$ which is a unitary operator on the state space of a two-qubit system. The controlled-CNOT is a quantum gate on three-qubit systems, which is known Toffoli gate. The third input qubit of a Toffoli gate will be flipped only when the first and the second input qubits are simultaneously activated.

A set of quantum gates is universal if any unitary gate which acts on arbitrary number of qubits can be implemented by the gates from the set. Combining unitary gates on single qubit, the CNOT gate is universal for quantum computing [72]. The Toffoli gate is universal if Hadamard gate can be used as a kind of free resource [73]. A Toffoli gate can be implemented by a collection of two-qubit gates. It turns out that five tow-qubit gates are necessary for the implementation [74].

One reason that quantum computer will have speed advantage on computation is that quantum state can be in superposition. The superposition of quantum states provides the possibility of realizing real parallelism computing, thereby speeding up the computation. We consider a general quantum register composed of n qubits. Suppose each qubit of the register is initialized in the state $|0\rangle$. By applying Hadamard gate on each qubit, the state of the register can be transformed to $|\Psi_n\rangle = |+\rangle \times \cdots \otimes |+\rangle$. The state $|\Psi_n\rangle$ can be equivalently written as

$$|\Psi_n\rangle = \frac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n-1} |k\rangle, \tag{2.19}$$

which is in a superposition of 2^n basis states. Suppose the unitary U_f standards for a quantum circuit of realizing the transformation $U_f : |k\rangle|0\rangle \to |k\rangle|f(k)\rangle$ where the first register contains the input state and the second one is used to store the computational result. Taking the superposition state $|\Psi_n\rangle$ as an input of the circuit, the final state of the registers would be $|f(\Psi_n)\rangle = \frac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n-1} |k\rangle|f(k)\rangle$. The output register simultaneously contains 2^n results of the function $f(k)$. It is amazing that we get exponential many results of the function through only one run of the circuit! By measuring the first register in the standard basis, the output register would be in the state $|f(k)\rangle$ if the outcome k was observed. Although a specific result can only be obtained probabilistically, the quantum superposition theory provides the possibility for achieving dramatic improvement on computational speed. One of the main tasks is to design quantum algorithm to make the measurement probability of observing the target result as high as possible. This is possible at least in some specific applications. One successful example is Shor's quantum algorithm for factoring large numbers [17].

The pure state of a general n-qubit system can be written as $|\psi\rangle = \sum_{k=0}^{2^n-1} \alpha_k |k\rangle$ where $\alpha_k \in \mathbb{C}$ and $\sum_{k=0}^{2^n-1} |\alpha_k|^2 = 1$. Thus, the representation of an n-qubit quantum system on a classical computer requires the storage of 2^n complex coefficient numbers. Note that a classical n-bit system only represents a number of binary length n. This is the main reason that it is quite inefficient to simulate quantum system on classical computers.

2.3.3 Quantum entanglement

Quantum entanglement is a "spooky" feature of quantum mechanics. Entanglement phenomenon can exist between groups of particles even when the particles are separated by a large distance [21]. To illustrate the phenomenon of entanglement, let us consider a quantum system of two qubits which is in the state

$$|\beta_{00}\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle). \tag{2.20}$$

We independently measure the subsystems in the computational basis. Although it is known that the two subsystems are simultaneously in the same state 0 or 1, we could not deterministically predict the results of the measurements. Any attempt to determine the state of one subsystem will destroy the knowledge of another subsystem. The observations contradict with the local realism principle of classical physics. This phenomenon was firstly recognized by Einstein, Podolsky and Rosen in the well-known EPR paper [31]. Schrödinger named the phenomenon as *entanglement* [32].

The entanglement illustrated in Eq. (2.20) is a purely entangled state which exists within a two-qubit system. In fact, quantum entanglement can exist between multipartite quantum system which is in a mixed state. We consider a bipartite quantum system which is composed of two subsystem A and B. Suppose the joint system $A \otimes B$ is in the state ρ_{AB}. If we ignore the subsystem B and only consider the subsystem A, the state ρ_A of the subsystem A is described by the partial trace of density operator ρ_{AB} over state space B, which is denoted as $\rho_A = tr_B(\rho_{AB})$. The partial trace is defined as $tr_B(\rho_{AB}) \equiv \sum_k \langle k|\rho_{AB}|k\rangle$ where $\{|k\rangle\}$ is an orthonormal basis of the state space of system B. Similarly, the state ρ_B of the subsystem B is $\rho_B = tr_A(\rho_{AB})$. If the state of the joint system can be written as $\rho_{AB} = \rho_A \otimes \rho_B$, we say that the joint system is in a *product state*. The joint system is in a *separable state* if the state ρ_{AB} can be written as

$$\rho_{AB} = \sum_k p_k \rho_A^k \otimes \rho_B^k, \tag{2.21}$$

which means that the joint system is in the product state $\rho_A^k \otimes \rho_B^k$ with probability p_k. If the state of the system cannot be written as the form in Eq. (2.21), we say that the bipartite system is *entangled* [21]. Operationally, quantum entanglement is a resource that could not be created via local operations and classical communication (LOCC) [75].

A class of important entangled two-qubit states are Bell states which are also known as EPR pairs. One of the Bell states is defined in Eq. (2.20). The others are as follows:

$$
\begin{aligned}
|\beta_0 1\rangle =& \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle), \\
|\beta_1 0\rangle =& \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle), \\
|\beta_1 1\rangle =& \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle).
\end{aligned}
$$

Bell states are not only maximally entangled but also of maximal nonlocality.

2.4 Bipartite nonlocality

The nonlocality between two participants, usually referred as bipartite nonlocality, is the basis for exploiting more complex nonlocality. Bipartite nonlocality has been extensively studied in the last five decades. We will give a technical introduction on bipartite nonlocality in this section.

2.4.1 Local hidden variable model of a bipartite scenario

We consider a classical scenario where two participants, say Alice and Bob, are separated. Suppose Alice receives an input information labelled by x. Then, she performs a strategy based on the input information and obtains an output labelled by a. Bob plays a similar role as Alice. Suppose the corresponding input and output of Bob are labelled by y and b, respectively. Let $p(a, b|x, y)$ be the probability that Alice and Bob obtain outputs a and b while their inputs are x and y, respectively. The statistical characteristics of this scenario is completely described by the conditional probability $p(a, b|x, y)$, which is also known as the correlation between the two participants. The scenario is depicted in Figure 2.2.

Einstein's theory of local realism is the combination of the locality principle and the reality principle, which is a fundamental feature of classical mechanics. According to the local realism theory, the action at one participant could not influence the output of the separated participant, which implies that the output statistics of

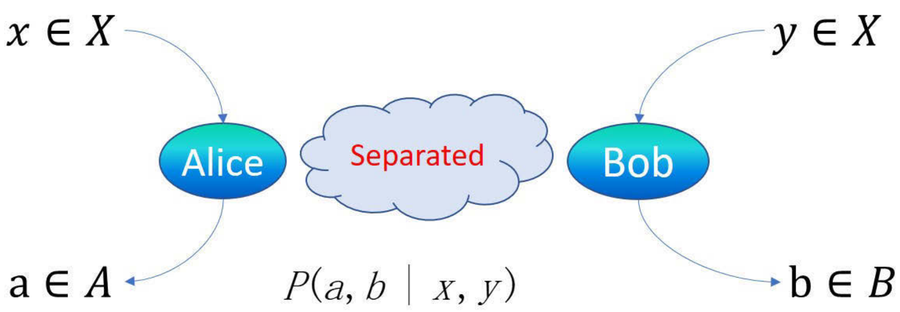

Fig. 2.2: The standard bipartite nonlocality test scenario.

Alice and Bob should be independent. However, there is an argument that there may be inaccessible variables which could influence the correlations between the outputs. John Stewart Bell mathematically formulized those inaccessible variables as a single variable, which is also known hidden variable [33]. With the supplement by Bell, the outputs of the participants are independent to each other and they are only determined by the value of the hidden variable and the corresponding input. Suppose the value of the hidden variable is denoted by λ. Then, the local realism principle implies that it should have

$$p(a, b|x, y, \lambda) = p(a|x, \lambda)p(b|y, \lambda). \tag{2.22}$$

Suppose $p(\lambda)$ is the probability of the hidden variable having value λ. Thus, the correlation $p(a, b|x, y)$ between Alice and Bob should be equivalently written as the following decomposition

$$p(a, b|x, y) = \sum_{\lambda} p(\lambda)p(a|x, \lambda)p(b|y, \lambda). \tag{2.23}$$

The mathematical model described in Eq. (2.23) is known as local hidden variable model (LHVM) of the scenario. With the supplemented hidden variable, the LHVM is consistent with the local realism theory. Conversely, any prediction of the scenario which is consistent with the local realism theory should admit a LHVM. Otherwise, if there is a correlation generated from the scenario which does not admit any LHVM, it would indicate that either the locality principle or the realism principle does not hold true.

For the scenario discussed above, we image that each received input indicates a measurement operation and the output is the outcome of the corresponding measurement. To consider the simplest scenario, we set a constrict that each participant performs a dichotomic measurement chosen from two possible measurement settings. Suppose $x \in \{x_0, x_1\}$ is the measurement setting for Alice and that for Bob is $y \in \{y_0, y_1\}$. The possible two outcomes of a measurement operation are labelled by $+1$ and -1. Let $E(x, y)$ be the expectation value of the product of Alice and Bob's measurement outcomes on condition that they choose the measurement settings x and y, respectively. Namely, $E(x, y) \equiv \sum_{a,b} a * b * p(a, b|x, y)$. As the prediction admits the LHVM described in Eq. (2.23), the expectation value can be equivalently rewritten as

$$E(x, y) = \sum_{\lambda} p(\lambda)E(x|\lambda)E(y|\lambda), \tag{2.24}$$

where $E(x|\lambda) \equiv \sum_a a * p(a|x, \lambda)$ and $E(y|\lambda) \equiv \sum_b b * p(b|y, \lambda)$. Due to $a, b \in \{+1, -1\}$, it implies that $|E(x|\lambda)| \leq 1$ and $|E(y|\lambda)| \leq 1$ which can result the following inequality

$$E(x_0|\lambda)E(y_0|\lambda) + E(x_0|\lambda)E(y_1|\lambda) + E(x_1|\lambda)E(y_0|\lambda) - E(x_1|\lambda)E(y_1|\lambda) \leq 2.$$

Multiplying the probability $p(\lambda)$ and then sum up them over all possible λ on both side of the above inequality, we will have the following inequality

$$E(x_0, y_0) + E(x_0, y_1) + E(x_1, y_0) - E(x_1, y_1) \leq 2. \tag{2.25}$$

The inequality in Eq. (2.25) is known as CHSH inequality, named after its inventors [34]. Any prediction based on local realism theory, namely it admits a LHVM, would satisfy the CHSH inequality.

2.4.2 *Bipartite quantum correlations and the violation of LHVM*

In the scenario described in Figure 2.2, suppose Alice and Bob share a bipartite quantum state ρ_{AB}. Alice performs a quantum measurement described by the measurement operators $\{M_a^x\}$ where x stands for the the measurement setting and a indicates the measurement outcome. The corresponding measurement operators of Bob are N_b^y. According to the theory of quantum mechanics, a quantum correlation can be generated from the scenario as follows

$$p(a, b|x, y) = tr((M_a^x \otimes N_b^y)\rho_{AB}). \tag{2.26}$$

Quantum correlations can violate the CHSH inequality, thereby indicating that quantum mechanics is nonlocal! An example for demonstrating the nonlocality of quantum mechanics is the EPR state $|\Phi\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$ of a two-qubit system. Suppose each of Alice and Bob owns a qubit of the two-qubit system. We consider dichotomic projective measurements in the scenario. Recall that a measurement observable on a single qubit system with eigenvalues being ± 1 can be represented by a unit vector in $\mathbb{R}^3$. Suppose Alice and Bob perform measurements described by the unit vectors $\vec{x}, \vec{y} \in \mathbb{R}^3$, respectively. A simple calculation shows that $E(\vec{x}, \vec{y}) = -(\vec{x}, \vec{y})$. Suppose $x \in \{x_0, x_1\}$ and $y \in \{y_0, y_1\}$. We set Alice's measurement settings such that $\vec{x_0}$ is orthogonal to $\vec{x_1}$. Further let $\vec{y_0} = -(\vec{x_0} + \vec{x_1})/\sqrt{2}$ and $\vec{y_1} = -(\vec{x_0} - \vec{x_1})/\sqrt{2}$. Then, the combination of the expectations in the left side of the CHSH inequality is

$$\begin{aligned}
& E(x_0, y_0) + E(x_0, y_1) + E(x_1, y_0) - E(x_1, y_1) \\
=& -(\vec{x_0}, \vec{y_0}) - (\vec{x_0}, \vec{y_1}) - (\vec{x_1}, \vec{y_0}) + (\vec{x_1}, \vec{y_1}) \\
=& \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2}} \\
=& 2\sqrt{2}.
\end{aligned} \tag{2.27}$$

Surprisingly, the result is $2\sqrt{2}$ which means that the CHSH inequality in Eq. (2.25) is violated! Thus, the predictions generated from scenario with the quantum resource $|\Phi\rangle$ does not admit a LHVM any more.

This observation indicates that the theory of quantum mechanics is not consistent with the theory of local realism. Therefore, quantum mechanics is nonlocal.

3. RELATIONSHIP BETWEEN ENTANGLEMENT AND NONLOCALITY OF A BIPARTITE QUANTUM SYSTEM

Entanglement and nonlocality are two of the most fundamental characteristics of quantum mechanics [21, 35]. Beside the fundamental significance for quantum mechanics, they are core inherent reasons that make quantum information processing tasks having great advantages over their classical counterparts [68]. The relationship between quantum entanglement and nonlocality is always of hot research interests.

In this chapter, we firstly considered the question whether a collection of quantum measurement settings is the best one for different quantum states in perspective of stimulating the most nonlocality. Note that the optimal measurement setting for stimulating the most nonlocality of a quantum state plays a significant role in practice. In many quantum information processing tasks, different quantum resources are also involved. It will take more effort to prepare the nonlocality test settings for different quantum resources. Thus, it is of practical significance if there are some quantum resources where the nonlocality could be optimally stimulated by the same nonlocality test setting.

Secondly, we quantitatively exploit the relationship between entanglement and nonlocality. To fully figure out the relationship between quantum nonlocality and entanglement is of great significance in perspective of understanding the nature. The qualitative relationship has been extensively studied in the last three decades. However, the quantitative relationship is not clear. This is the main motivation of this chapter.

The chapter is organized as follows. In Section 3.1, we give a brief introduction to the quantitative measures of quantum entanglement and quantum nonlocality. Further, we get an analytical expression of the quantum setting which can optimal test the nonlocality of a general two-qubit state. In Section 3.2, we exploit the condition that two different general two-qubit states could have the same optimal nonlocality test setting. In Section 3.3, we figure out all the pairs of two-qubit pure states which have the same optimal nonlocality test setting. In Section 3.4, we find out that the nonlocality of a general two-qubit state is upper bounded by a function of the entanglement. Note that this is an independent research with Verstraete's work. Based on the outcomes in Sections 3.2 and 3.3, we further find the necessary and sufficient condition for a two-qubit state to achieve the upper bound which is specified by its entanglement.

3.1 Measures of entanglement and nonlocality

As quantum entanglement and nonlocality are indispensable resources for quantum information processing tasks, quantifying the amount of entanglement and nonlocality that are contained in a bipartite quantum system are of both theoretical and practical significance.

In this section, we give a brief introduction on the quantitative measures of quantum entanglement and quantum nonlocality of an arbitrary two-qubit states, respectively. We also find out the specific quantum measurement setting that stimulates the most nonlocality from a quantum state.

3.1.1 Entanglement of two-qubit state

Entanglement of a bipartite quantum system $A \otimes B$ is quantified by *entanglement of formation* [76], denoted as $E(\cdot)$. In the following discussions, we refer "entanglement of formation" simply as "entanglement".

The entanglement $E(\psi)$ of a bipartite pure state $|\psi\rangle$ is the asymptotic number of standard singlets required to locally prepare the state. It also equals the von Neumann entropy of either of the two subsystems. Namely,

$$E(\psi) = -tr(\rho_A log_2 \rho_A) = -tr(\rho_B log_2 \rho_B), \tag{3.1}$$

where $\rho_A = tr_B(|\psi\rangle\langle\psi|)$ and $\rho_B = tr_A(|\psi\rangle\langle\psi|)$ are the corresponding density operators of two subsystems, respectively. For a general bipartite quantum system, $E(\psi)$ is a quantity that ranges from zero to $\log_2 N$ where N is the dimension of the subsystem. $E(\psi)$ reaches $\log_2 N$ for the maximally entangled state $|\Omega\rangle \equiv \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} |k\rangle|k\rangle$

while it is zero for any product state. In the case of two-qubit system, the dimension $N = 2$ and the entanglement ranges from 0 to 1.

The entanglement of mixed states is much more complicated. The entanglement of the bipartite state ρ_{AB} is defined as the least expected entanglement of any ensemble of pure states that realizes the state ρ_{AB}. That is

$$E(\rho_{AB}) = min \sum_k p_k E(\psi_k), \tag{3.2}$$

where the minimization is over all possible purely decomposition of ρ_{AB} such that $\rho_{AB} = \sum_k p_k |\psi_k\rangle\langle\psi_k|$.

The entanglement of a two-qubit system is closely related to *concurrence*, which is a quantity proposed by Hill and Wootters [77]. The concurrence of a two-qubit pure state $|\psi\rangle$ is defined as

$$C(\psi) = |\langle\psi|\tilde{\psi}\rangle|, \tag{3.3}$$

where $|\tilde{\psi}\rangle = (\sigma_y \otimes \sigma_y)|\psi^*\rangle$. Note that $|\psi^*\rangle$ is the complex conjugate of $|\psi\rangle$. It is trivial to find out that the entanglement of a two-qubit pure state and its concurrence is related by the following relation

$$E(\psi) = h(\frac{1 + \sqrt{1 - C(\psi)^2}}{2}), \tag{3.4}$$

where $h(\cdot)$ is a binary function defined as $h(x) \equiv -x \log_2 x - (1-x)\log_2(1-x)$ with $x \in [0, 1]$. One usually denotes that $\log_2 0 \equiv 0$ in order to keep the completeness of the definition of $h(x)$. The function $h(x)$ is known as Shannon's binary entropy function [78].

Later, Wootters showed that the formula for the entanglement of two-qubit pure state in Eq. (3.4) also applies for that of mixed state [79]. To achieve this, he derived an analytical expression for the concurrence of a two-qubit state ρ. Define $\tilde{\rho} \equiv (\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y)$ as the spin-flipped state of ρ where ρ^* is the complex conjugate of the density operator ρ. Then, the concurrence of ρ can be equivalently written as

$$C(\rho) = max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}, \tag{3.5}$$

where $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$ are the eigenvalues of the Hermitian matrix $\sqrt{\rho\tilde{\rho}}$. Finally, the entanglement of a general two-qubit state ρ can be written as

$$E(\rho) = h(\frac{1 + \sqrt{1 - C(\rho)^2}}{2}). \tag{3.6}$$

The key of evidencing this result is that Wootters noticed the existence of a special decomposition of the general two-qubit state. We conclude the decomposition in Lemma 1.

Lemma 1. *Suppose ρ is an arbitrary density operator of a two-qubit system. There is an ensemble of pure states $\{p_k, |\psi_k\rangle\}$ for ρ such that the concurrence $C(\psi_k) = C(\rho)$ for each state $|\psi_k\rangle$.*

Note that the concurrence of a density operator is a quantity ranging from 0 to 1. The separable states correspond to concurrence 0 and the maximally entangled states correspond to concurrence 1. The entanglement $E(\rho)$ is monotonically increasing as $C(\rho)$ goes from 0 to 1. Therefore, concurrence can also act as a measure of entanglement in its own right.

3.1.2 Nonlocality of two-qubit state

We admit the standard bipartite scenario described in Section 2.4, which consist of two separated participants Alice and Bob. In a simplest scenario for generating bipartite quantum correlations, each participant performs a dichotomic measurement which is taken from two possible choices. We only consider projective measurements on single qubit systems where the outcomes are labelled by $+1$ and -1. Note that such a measurement can be completely described by an observable, which is a Hermitian on the state space $\mathcal{H}_2$. The observable can be equivalently represented by a unit vector in $\mathbb{R}^3$.

Suppose Alice and Bob share a two-qubit state ρ. The observables for Alice's measurement observables are denoted by A and A' while that of Bob are denoted by B and B'. Then, the corresponding CHSH inequality can be equivalently rewritten as

$$tr(\rho S) \leq 2, \tag{3.7}$$

where S is a CHSH operator of the form

$$S = A \otimes (B + B') + A' \otimes (B - B'). \tag{3.8}$$

A bipartite local state ρ admits the CHSH inequality for any possible CHSH operator S while it is nonlocal if there is a CHSH operator S such that the CHSH inequality can be violated. Thus, the violation of the CHSH inequality is a sufficient evidence that the state ρ is nonlocal.

Recall that a common choice for quantifying the nonlocality of a quantum state is through the maximal violation of the corresponding Bell inequality. Thus, the nonlocality of the two-qubit state ρ can be quantitatively defined as the maximal value of the CHSH expression. Namely,

$$\mathcal{N}(\rho) \equiv \max_{S} tr(\rho S), \tag{3.9}$$

where the maximum is over all possible CHSH operators. In the following discussion, we refer the nonlocality of a state as the quantity $\mathcal{N}(\cdot)$. We also refer the CHSH operator that can achieve the nonlocality $\mathcal{N}(\rho)$ as the optimal CHSH operator of state ρ.

It is obvious that the measure $\mathcal{N}(\cdot)$ of bipartite nonlocality is a convex function of bipartite density operators on $\mathcal{H}_2^{\otimes 2}$. Suppose ρ^{AB} is a density operator that can be generated from the ensemble $\{q_k, \rho_k^{AB}\}$, namely $\rho^{AB} = \sum_k q_k \rho_k^{AB}$. Let S be the optimal CHSH operator of the state ρ^{AB}. Then, the convexity of nonlocality can be convinced by the following equation

$$\mathcal{N}\big(\sum_k q_k \rho_k^{AB}\big) = \sum_k q_k tr(\rho_k^{AB} S) \leq \sum_k q_k \mathcal{N}(\rho_k^{AB}). \tag{3.10}$$

The equality in Eq. (3.10) holds if and only if the equation $\mathcal{N}(\rho_k^{AB}) = \mathcal{N}(\rho^{AB})$ applies for all constituent state ρ_k^{AB}.

3.1.3 The optimal CHSH operator

Horodecki et al. got an analytical expression for the nonlocality of a general two-qubit state [45]. In this subsection, we review the process of analyzing the nonlocality and further work out the mathematical expression of the corresponding optimal CHSH operator.

Any density operator ρ of a two-qubit quantum system can be represented by the combination of the identity operator and the generators of the $SU(2)$ algebra [80] as follows

$$\rho = \frac{1}{4}(I \otimes I + \vec{r} \cdot \vec{\sigma} \otimes I + I \otimes \vec{s} \cdot \vec{\sigma} + \sum_{j,k=1}^{3} T_{jk} \sigma_j \otimes \sigma_k), \tag{3.11}$$

where $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is the vector of Pauli matrices and the coefficient $T_{jk} = tr(\sigma_j \otimes \sigma_k \rho)$ is the element of a 3×3 real matrix T. The vectors $\vec{r}$ and $\vec{s}$ only determine the properties of the two subsystems, respectively. The global properties between the joint system are contained in the matrix T. Thus, we call matrix T the correlation matrix of the two-qubit state ρ.

Note that the measurement observable A of a qubit system can be represented by a unit column vector $\vec{a} \in \mathbb{R}^3$ such that $A = \vec{a} \cdot \vec{\sigma}$. Let $\vec{a}$,$\vec{a'}$,$\vec{b}$ and $\vec{b'}$ be the corresponding vectors of the measurement observables A, A', B and B', respectively. Then, the expectation value of the joint measurement observable $A \otimes B$ can be written as

$$tr(A \otimes B\rho) = \sum_{j,k=1}^{3} a_j T_{jk} b_k = \langle a|T|b\rangle. \tag{3.12}$$

Here we abuse the Dirac notation $|a\rangle$, which usually stands for the pure state of a quantum system, for the unit column vector $\vec{a}$. In the following discussions, we will interchangeably use the two kinds of notations based on the convenience of expression.

Let $\vec{b}+\vec{b'} = 2\cos\theta\vec{c}$ and $\vec{b}-\vec{b'} = 2\sin\theta\vec{c'}$ for some $\theta \in [0, \pi)$ and $\vec{c}, \vec{c'} \in \mathbb{R}^3$ are unit vectors. Note that the vectors $\vec{c}$ and $\vec{c'}$ are orthogonal. Let $T^T T = \sum_{k=1}^{3} \lambda_k |\mu_k\rangle\langle\mu_k|$ be the spectral decomposition of the Hermitian matrix $T^T T$. With out loss of generality, suppose the eigenvalues λ_k are in the nonincreasing order, namely $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq 0$. Then, we can get inequalities as follows

$$\begin{aligned}
tr(S\rho) &= tr(A \otimes (B + B')\rho) + tr(A' \otimes (B - B')\rho) \\
&= 2\cos\theta\langle a|T|c\rangle + 2\sin\theta\langle a'|T|c'\rangle \\
&\leq 2\sqrt{(\langle a|T|c\rangle)^2 + (\langle a'|T|c'\rangle)^2} \qquad (3.13) \\
&\leq 2\sqrt{\|T|c\rangle\|^2 + \|T|c'\rangle\|^2} \qquad (3.14) \\
&\leq 2\sqrt{\lambda_1 + \lambda_2}. \qquad (3.15)
\end{aligned}$$

The inequality in Eq. (3.15) is with equation when $|c\rangle = \eta|\mu_1\rangle$ and $|c'\rangle = \eta'|\mu_2\rangle$ with $\eta, \eta' \in \{+1, -1\}$ being signs. In this case, $\|T|c\rangle\|^2 = \langle c|T^T T|c\rangle = \lambda_1$ and $\|T|c'\rangle\|^2 = \langle c'|T^T T|c'\rangle = \lambda_2$. The equality of Eq. (3.14) holds when $|a\rangle = \delta\frac{T|c\rangle}{\|T|c\rangle\|}$ and $|a'\rangle = \delta'\frac{T|c'\rangle}{\|T|c'\rangle\|}$ with signs $\delta, \delta' \in \{+1, -1\}$. And the equality in Eq. (3.13) holds when $\cos\theta = \frac{\langle a|T|c\rangle}{\sqrt{\langle a|T|c\rangle^2+\langle a'|T|c'\rangle^2}}$ and $\sin\theta = \frac{\langle a'|T|c'\rangle}{\sqrt{\langle a|T|c\rangle^2+\langle a'|T|c'\rangle^2}}$. The upper bound

$2\sqrt{\lambda_1+\lambda_2}$ of $tr(S\rho)$ can be achieved when the equalities in Eqs. (3.13)-(3.15) hold simultaneously. Namely, $tr(S\rho)=2\sqrt{\lambda_1+\lambda_2}$ when $\cos\theta=\frac{\delta\sqrt{\lambda_1}}{\sqrt{\lambda_1+\lambda_2}}$, $\sin\theta=\frac{\delta'\sqrt{\lambda_2}}{\sqrt{\lambda_1+\lambda_2}}$, $|a\rangle=\delta\eta\frac{T|\mu_1\rangle}{\sqrt{\lambda_1}}$, $|a'\rangle=\delta'\eta'\frac{T|\mu_2\rangle}{\sqrt{\lambda_2}}$, $|c\rangle=\eta|\mu_1\rangle$ and $|c'\rangle=\eta'|\mu_2\rangle$. Thus, the nonlocality of state ρ is $\mathcal{N}(\rho)=2\sqrt{\lambda_1+\lambda_2}$. And the corresponding optimal CHSH operator of state ρ is

$$
\begin{aligned}
S &= 2\cos\theta A\otimes C + 2\sin\theta A'\otimes C' \\
&= 2\delta\sqrt{\frac{\lambda_1}{\lambda_1+\lambda_2}}\Big(\frac{\delta\eta}{\sqrt{\lambda_1}}T\vec{\mu_1}\Big)\cdot\vec{\sigma}\otimes(\eta\vec{\mu_1})\cdot\vec{\sigma}+ \\
&\quad 2\delta'\sqrt{\frac{\lambda_2}{\lambda_1+\lambda_2}}\Big(\frac{\delta'\eta'}{\sqrt{\lambda_2}}T\vec{\mu_2}\Big)\cdot\vec{\sigma}\otimes(\eta'\vec{\mu_2})\cdot\vec{\sigma} \\
&= \frac{2}{\sqrt{\lambda_1+\lambda_2}}(T\vec{\mu_1}\cdot\vec{\sigma}\otimes\vec{\mu_1}\cdot\vec{\sigma}+T\vec{\mu_2}\cdot\vec{\sigma}\otimes\vec{\mu_2}\cdot\vec{\sigma}).
\end{aligned}
\tag{3.16}
$$

Let $w_{jk}\equiv\frac{1}{4}tr(S\sigma_j\otimes\sigma_k)$ be the Pauli coefficients of the optimal CHSH operator S. Namely, $S=\sum_{j,k=1}^{3}w_{jk}\sigma_j\otimes\sigma_k$. Thus, the optimal CHSH operator S of state ρ is uniquely corresponding to a 3×3 real matrix $W=(w_{jk})_{3\times3}$. Taking the standard basis, the matrix W can be written as

$$
\begin{aligned}
W &= \sum_{j,k=1}^{3} w_{jk}|j\rangle\langle k| \\
&= \frac{2}{\sqrt{\lambda_1+\lambda_2}}\sum_{j,k=1}^{3}((T|\mu_1\rangle)_j(|\mu_1\rangle)_k+(T|\mu_2\rangle)_j(|\mu_2\rangle)_k)|j\rangle\langle k| \\
&= \frac{2}{\sqrt{\lambda_1+\lambda_2}}T(|\mu_1\rangle\langle\mu_1|+|\mu_2\rangle\langle\mu_2|).
\end{aligned}
$$

We conclude the above analysis as the following lemma, which is the main result of this section.

Lemma 2. *Suppose ρ is an arbitrary two-qubit state with correlation matrix T and the eigenvalues in the spectral decomposition $T^TT=\sum_{k=1}^{3}\lambda_k|\mu_k\rangle\langle\mu_k|$ are in the nonincreasing order. Then, the nonlocality of state ρ is $\mathcal{N}(\rho)=2\sqrt{\lambda_1+\lambda_2}$. The optimal CHSH operator of state ρ is $S=\sum_{j,k=1}^{3}w_{jk}\sigma_j\otimes\sigma_k$ which is uniquely specified by the corresponding Pauli coefficients matrix*

$$
W=\frac{2}{\sqrt{\lambda_1+\lambda_2}}T(|\mu_1\rangle\langle\mu_1|+|\mu_2\rangle\langle\mu_2|).
\tag{3.17}
$$

3.2 Two different states having the same optimal CHSH operator

In this section, we research the question whether the nonlocality of different quantum states can be stimulated by the same quantum nonlocality test setting. Let T and F be correlation matrices of two-qubit states ρ and ϱ, respectively. We try to work out the condition that the optimal CHSH operators of the states ρ and ϱ can be the same.

Suppose the singular value decomposition of T is $T = UDV$ where $U = \sum_{k=1}^{3} |\mu_k\rangle\langle k|$, $V = \sum_{k=1}^{3} |k\rangle\langle \nu_k|$ are orthogonal matrices and $D = \sum_{k=1}^{3} t_k|k\rangle\langle k|$ is a diagonal matrix. Then, we have $T = \sum_{k=1}^{3} t_k|\mu_k\rangle\langle v_k|$ and $T^T T = \sum_{k=1}^{3} t_k^2|v_k\rangle\langle v_k|$. With out loss of generality, suppose $|t_1| \geq |t_2| \geq |t_3|$. According to Lemma 2, the corresponding Pauli coefficients matrix of the optimal CHSH operator for state ρ can be written as

$$W = \frac{2}{\sqrt{t_1^2 + t_2^2}}(t_1|\mu_1\rangle\langle\nu_1| + t_2|\mu_2\rangle\langle\nu_2|). \tag{3.18}$$

Suppose the singular value decomposition of F is $F = PEQ$ where $P = \sum_{k=1}^{3} |\alpha_k\rangle\langle k|$, $Q = \sum_{k=1}^{3} |k\rangle\langle\beta_k|$ and $E = \sum_{k=1}^{3} f_k|k\rangle\langle k|$. Further suppose $|f_k|$ are in the nonincreasing order. Similarly, the corresponding matrix of the optimal CHSH operator for state ϱ can be written as

$$R = \frac{2}{\sqrt{f_1^2 + f_2^2}}(f_1|\alpha_1\rangle\langle\beta_1| + f_2|\alpha_2\rangle\langle\beta_2|). \tag{3.19}$$

The preset condition that the optimal CHSH operators of two-qubit states ρ and ϱ are the same is equivalent to the relation $W = R$. Let $\cos t = \frac{t_1}{\sqrt{t_1^2+t_2^2}}$, $\sin t = \frac{t_2}{\sqrt{t_1^2+t_2^2}}$, $\cos f = \frac{f_1}{\sqrt{f_1^2+f_2^2}}$ and $\sin f = \frac{f_2}{\sqrt{f_1^2+f_2^2}}$. Then, the relation $W = R$ can be equivalently written as

$$\cos t|\mu_1\rangle\langle\nu_1| + \sin t|\mu_2\rangle\langle\nu_2| = \cos f|\alpha_1\rangle\langle\beta_1| + \sin f|\alpha_2\rangle\langle\beta_2|. \tag{3.20}$$

Let $M = (m_{kj})$ be a 2×2 matrix where $m_{kj} = \langle\mu_k|\alpha_j\rangle\langle\beta_j|\nu_k\rangle$. Then, some equations can be derived from Eq. (3.20) as follows

$$\cos t = m_{11}\cos f + m_{12}\sin f, \tag{3.21}$$

$$\sin t = m_{21}\cos f + m_{22}\sin f, \tag{3.22}$$

$$\cos f = m_{11}\cos t + m_{21}\sin t, \tag{3.23}$$

$$\sin f = m_{12}\cos t + m_{22}\sin t. \tag{3.24}$$

Denote $|t\rangle \equiv \cos t|0\rangle + \sin t|1\rangle$ and $|f\rangle \equiv \cos f|0\rangle + \sin f|1\rangle$. The Eqs. (3.21)-(3.24) can be equivalently written as

$$|t\rangle = M|f\rangle \text{ and } |f\rangle = M^T|t\rangle. \tag{3.25}$$

It follows that $|t\rangle = MM^T|t\rangle$ and $|f\rangle = M^TM|f\rangle$ for all possible vectors $|t\rangle$ and $|f\rangle$. Thus, it must have $M^TM = MM^T = I$, which means M is an orthogonal matrix. Namely, $m_{11}^2 + m_{12}^2 = 1$ and $m_{21}^2 + m_{22}^2 = 1$.

However, we note that

$$m_{11}^2 + m_{12}^2 = (\langle\mu_1|\alpha_1\rangle\langle\beta_1|\nu_1\rangle)^2 + (\langle\mu_1|\alpha_2\rangle\langle\beta_2|\nu_1\rangle)^2 \leq 1, \tag{3.26}$$

and

$$m_{21}^2 + m_{22}^2 = (\langle\mu_2|\alpha_1\rangle\langle\beta_1|\nu_2\rangle)^2 + (\langle\mu_2|\alpha_2\rangle\langle\beta_2|\nu_2\rangle)^2 \leq 1. \tag{3.27}$$

Thus, the equalities in Eqs. (3.26) and (3.27) must hold simultaneously. The conditions that the equalities hold true are $|\mu_k\rangle = \delta_k|\alpha_k\rangle, |\nu_k\rangle = \delta_k'|\beta_k\rangle$ for $k = 1, 2$ or $|\mu_1\rangle = \delta_1|\alpha_2\rangle, |\mu_2\rangle = \delta_2|\alpha_1\rangle, |\nu_1\rangle = \delta_1'|\beta_2\rangle, |\mu_2\rangle = \delta_2|\alpha_1\rangle$ where $\delta_k, \delta_k' \in \{\pm 1\}$ are signs. With out loss of generality, we can set $\delta_k = \delta_k' = 1$ and pat the signs into the singular values. In the former case of conditions, it follows that $|\mu_k\rangle = |\alpha_k\rangle, |\nu_k\rangle = |\beta_k\rangle$ for $k = 1, 2, 3$ and $\cos t = \cos f$, $\sin t = \sin f$. Hence, the correlation matrices of states ρ and ϱ are related as follows:

$$\begin{aligned} T &= \sum_{k=1}^{3} t_k|\mu_k\rangle\langle\nu_k| \\ &= \sqrt{t_1^2 + t_2^2}(\cos t|\alpha_1\rangle\langle\beta_1| + \sin t|\alpha_2\rangle\langle\beta_2|) + t_3|\alpha_3\rangle\langle\beta_3| \\ &= \sqrt{\frac{t_1^2 + t_2^2}{f_1^2 + f_2^2}}(f_1|\alpha_1\rangle\langle\beta_1| + f_2|\alpha_2\rangle\langle\beta_2|) + t_3|\alpha_3\rangle\langle\beta_3|. \end{aligned} \tag{3.28}$$

In the later case of conditions, we get the same relation as that of the former case which is shown in Eq. (3.28).

A more general case is that $|t_1|$, $|t_2|$ and $|t_3|$ are in a specified order, say decreasing order, while $|f_1|$, $|f_2|$ and $|f_3|$ are in an arbitrary order. Without loss of generality, suppose $|f_2|$ is the minimum in $\{|f_k|\}$. With similar analysis, we find out that the relation $W = R$ can be equivalently written as

$$T = \sqrt{\frac{t_1^2 + t_2^2}{f_1^2 + f_2^2}}(f_1|\alpha_1\rangle\langle\beta_1| + f_3|\alpha_3\rangle\langle\beta_3|) + t_3|\alpha_2\rangle\langle\beta_2|. \tag{3.29}$$

Obviously, the absolute values of correlation matrices T's and F's singular values are in the same order.

Based on the above analysis, we can conclude the conditions for the situation that two different general two-qubit states have the same optimal CHSH operator in the following theorem.

Theorem 1. *Suppose T is the correlation matrix of the two-qubit state ρ and F is that of the two-qubit state ϱ. Let t_1, t_2, t_3 and f_1, f_2, f_3 be singular values of the correlation matrices T and F, respectively. Then, the states ρ and ϱ have a same optimal CHSH operator if and only if they satisfy three conditions which are listed as follows:*

(1) T and F have the same orthogonal matrices in the singular value decompositions. Namely, the singular value decomposition of T and F can be written as

$$T = UDV \text{ and } F = UEV, \tag{3.30}$$

where $D = \sum_{k=1}^{3} t_k |k\rangle\langle k|$, $F = \sum_{k=1}^{3} f_k |k\rangle\langle k|$, U and V are orthogonal matrices.

(2) The absolute values of two sets of singular values, $\{|t_k|\}$ and $\{|f_k|\}$, are of the same order.

(3) Without loss of generality, suppose $\{|t_k|\}$ and $\{|f_k|\}$ are in the nonincreasing orders. Then, it should have

$$\frac{t_1}{f_1} = \frac{t_2}{f_2} = \sqrt{\frac{t_1^2 + t_2^2}{f_1^2 + f_2^2}}. \tag{3.31}$$

3.3 The collection of two-qubit pure states that share the same optimal CHSH operator

Recall that any mixed state can be viewed as an ensemble of pure states. Suppose ρ is an arbitrary two-qubit state which is generated from the ensemble $\{p_k, |\psi_k\rangle\}$. Namely, $\rho = \sum_k p_k |\psi_k\rangle\langle\psi_k|$ where $p_k \geq 0$ and $\sum_k p_k = 1$. The convexity of nonlocality indicates that

$$\mathcal{N}(\rho) \leq \sum_k p_k \mathcal{N}(\psi_k). \tag{3.32}$$

The equality holds if and only if the optimal CHSH operator of ρ also acts as the optimal CHSH operator of $|\psi_k\rangle$ for all k. In other words, it requires that the collection of pure states $\{|\psi_k\rangle\}$ have the same optimal CHSH operator.

In this section, we exploit the collection of two-qubit pure states which have the same optimal CHSH operator.

3.3.1 The role of local unitary operations

Suppose the two-qubit state ρ is shared by Alice and Bob. U_A and U_B are unitary operators which act on Alice's and Bob's subsystems, respectively. They can transform the state ρ into another state

$$\rho' = (U_A \otimes U_B)\rho(U_A \otimes U_B)^\dagger. \tag{3.33}$$

Suppose the optimal CHSH operators for ρ and ρ' are S and S', respectively. Then, it follows that

$$\begin{aligned}\mathcal{N}(\rho') &= tr(S'\rho') \\ &= tr((U_A \otimes U_B)^\dagger S'(U_A \otimes U_B)\rho) \\ &\leq \mathcal{N}(\rho) \\ &= tr(S\rho).\end{aligned}$$

Similarly, it has $tr(S\rho) \leq tr((U_A \otimes U_B)^\dagger S'(U_A \otimes U_B)\rho)$. Thus, the equality should holds, namely $tr(S\rho) = tr((U_A \otimes U_B)^\dagger S'(U_A \otimes U_B)\rho)$. Therefore, it should have $\mathcal{N}(\rho') = \mathcal{N}(\rho)$ and $S' = (U_A \otimes U_B)S(U_A \otimes U_B)^\dagger$. It also indicates that local unitary operations do not affect the nonlocality of the shared state.

Suppose the correlation matrices of the states ρ and ρ' are $T = (T_{kj})_{3\times 3}$ and $T' = (T'_{kj})_{3\times 3}$, respectively. Then, any element T'_{kj} of the correlation matrix T' can be equivalently rewritten as

$$\begin{aligned}T'_{kj} =& tr(\rho' \sigma_k \otimes \sigma_j) \\ =& tr(\rho(U_A^\dagger \sigma_k U_A \otimes U_B^\dagger \sigma_j U_B)) \\ =& \frac{1}{4}\sum_{k',j'=1}^{3} T_{k'j'} tr(\sigma_{k'} U_A^\dagger \sigma_k U_A) tr(\sigma_{j'} U_B^\dagger \sigma_j U_B).\end{aligned} \tag{3.34}$$

Let R_A and R_B be two matrices with elements defined as $(R_A)_{kk'} \equiv \frac{1}{2}tr(\sigma_k U_A \sigma_{k'} U_A^\dagger)$ and $(R_B)_{jj'} \equiv \frac{1}{2}tr(\sigma_j U_B \sigma_{j'} U_B^\dagger)$, respectively. It follows that $T'_{kj} = \sum_{k',j'=1}^{3}(R_A)_{kk'} T_{k'j'} (R_B)_{jj'} =$

$(R_A T R_B^T)_{kj}$. Thus, it has

$$T' = R_A T R_B^T. \tag{3.35}$$

Note that $SU(N)$ matrices have the completeness relation as follows [81]:

$$\sum_{j=1}^{N^2-1} (\sigma_j)_{ki}(\sigma_j)_{mn} = 2\Delta_{im}\Delta_{kn} - \frac{2}{N}\delta_{ki}\Delta_{mn}, \tag{3.36}$$

where $\Delta_{jk} = 1$ if $j = k$ and $\Delta_{jk} = 0$ otherwise. Applying the completeness relation in Eq. (3.36), it can be shown that R^A and R^B are orthogonal matrices.

We can conclude the above analysis as the following lemma.

Lemma 3. *Suppose Alice and Bob apply the local unitaries U_A and U_B on subsystems of the shared two-qubit state ρ, respectively. Suppose the correlation matrix of the state ρ is T. Then, the correlation matrix of the final state ρ' is*

$$T' = R_A T R_B^T, \tag{3.37}$$

where R_A and ${R_B}^T$ are two 3×3 orthogonal real matrices defined as

$$(R_A)_{kk'} \equiv \frac{1}{2} tr(\sigma_k U_A \sigma_{k'} U_A^\dagger), \tag{3.38}$$

and

$$(R_B)_{jj'} \equiv \frac{1}{2} tr(\sigma_j U_B \sigma_{j'} U_B^\dagger), \tag{3.39}$$

respectively.

3.3.2 The class of two-qubit pure state pairs with the same optimal CHSH operators

We consider a general two-qubit pure state $|\psi\rangle$ with correlation matrix T. Suppose the singular value decomposition of T is $T = R_A D R_B$ where D is a diagonal matrix and R_A, R_B are orthogonal matrices. Let U_A and U_B be the unitary operators that generate the orthogonal matrices R_A^T and R_B according to the definitions in Eqs. (3.38) and (3.39), respectively. According to Lemma 3, the correlation matrix of the state $(U_A \otimes U_B)|\psi\rangle$ is the diagonal matrix D. Namely, any two-qubit pure state can transformed into another pure state with diagonal correlation matrix via local unitary operations.

Suppose $|\varphi\rangle$ is a two-qubit pure state which has the same optimal CHSH operator with $|\psi\rangle$. Combining the Theorem 1, it is obviously that any two-qubit pure states $|\psi\rangle$ and $|\varphi\rangle$ can be simultaneously transformed into the states which have diagonal correlation matrices, by applying the same local unitary operations. Thus, we only need to look into the kind of two-qubit states with diagonal correlation matrices in order to analyze the class of two-qubit pure state pairs which have the same optimal CHSH operators.

Up to an ignorable global phase, a general two-qubit pure state can be equivalently written as

$$|\psi\rangle = a|00\rangle + (b_1 + ib_2)|01\rangle + (c_1 + ic_2)|10\rangle + (d_1 + id_2)|01\rangle,$$

where the variables are all real numbers that satisfy the unit condition $a^2 + b_1^2 + b_2^2 + c_1^2 + c_2^2 + d_1^2 + d_2^2 = 1$. The elements of the corresponding correlation matrix $T = (T_{ij})_{3\times 3}$ are

$$\begin{aligned}
T_{12} &= 2(-ad_2 - b_2c_1 + b_1c_2),\\
T_{13} &= 2(ac_1 - b_1d_1 - b_2d_2),\\
T_{21} &= 2(-ad_2 + b_2c_1 - b_1c_2),\\
T_{23} &= 2(-ac_2 - b_2d_1 + b_1d_2),\\
T_{31} &= 2(ab_1 - c_1d_1 - c_2d_2),\\
T_{32} &= 2(-ab_2 - c_2d_1 + c_1d_2),\\
T_{11} &= 2(ad_1 + b_1c_1 + b_2c_2),\\
T_{22} &= 2(-ad_1 + b_1c_1 + b_2c_2),\\
T_{33} &= 2(a^2 + d_1^2 + d_2^2) - 1.
\end{aligned}$$

By setting $T_{kj} = 0$ for all $k \neq j \in \{1, 2, 3\}$, we derive that any two-qubit pure state, of which the correlation matrix is diagonal, should be in one of the forms listed as follows:

$$|\Phi_{(\theta)}\rangle = \cos\theta|00\rangle + \sin\theta|11\rangle, \tag{3.40}$$

$$|\Omega_{(\theta)}\rangle = \cos\theta|01\rangle + \sin\theta|10\rangle, \tag{3.41}$$

$$|\Lambda_{(\theta,\delta)}\rangle = \cos\theta(|00\rangle + \delta|11\rangle)/\sqrt{2} + i\sin\theta(|01\rangle - \delta|10\rangle)/\sqrt{2}, \tag{3.42}$$

$$|\Pi_{(\theta,\delta)}\rangle = \cos\theta(|00\rangle + \delta|11\rangle)/\sqrt{2} + \sin\theta(|01\rangle + \delta|10\rangle)/\sqrt{2}, \tag{3.43}$$

where $\theta \in [0, \pi)$ and $\delta = \pm 1$. The corresponding correlation matrices are

$$T_\Phi(\theta) = \begin{bmatrix} \sin 2\theta & 0 & 0 \\ 0 & -\sin 2\theta & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

$$T_\Omega(\theta) = \begin{bmatrix} \sin 2\theta & 0 & 0 \\ 0 & \sin 2\theta & 0 \\ 0 & 0 & -1 \end{bmatrix},$$

$$T_\Lambda(\theta, \delta) = \begin{bmatrix} \delta \cos 2\theta & 0 & 0 \\ 0 & -\delta & 0 \\ 0 & 0 & \cos 2\theta \end{bmatrix},$$

$$T_\Pi(\theta, \delta) = \begin{bmatrix} \delta & 0 & 0 \\ 0 & -\delta \cos 2\theta & 0 \\ 0 & 0 & \cos 2\theta \end{bmatrix}.$$

Applying Theorem 1, we find out that there is no pair of two-qubit pure states which are of the different forms in Eqs. (3.40)-(3.43) and have the same optimal CHSH operator. For the pair $(|\Phi_{(\theta)}\rangle, |\Omega_{(\theta)}\rangle)$, the corresponding ratio is negative, which contradicts with the third condition in Theorem 1. Although matrices $T_\Phi(\theta)$ and $-T_\Omega(\theta)$ satisfy the conditions listed in Theorem 1, $-T_\Omega(\theta)$ is not a correlation matrix of any valid two-qubit pure state. If the pair $(|\Phi_{(\theta)}\rangle, |\Lambda_{(\theta,\delta)}\rangle)$ of states have the same optimal CHSH operators, it should have $\delta \sin 2\theta \cos 2\theta = 1$ which is impossible. The same reason stops the pairs $(|\Phi_{(\theta)}\rangle, |\Pi_{(\theta,\delta)}\rangle)$, $(|\Omega_{(\theta)}\rangle, |\Lambda_{(\theta,\delta)}\rangle)$ and $(|\Omega_{(\theta)}\rangle, |\Pi_{(\theta,\delta)}\rangle)$ to have the same optimal CHSH operators. If the pair $(|\Lambda_{(\theta,\delta)}\rangle, |\Pi_{(\theta,\delta)}\rangle)$ have the same optimal CHSH operators, it follows that $\cos^2 2\theta = 1$, namely $\sin\theta = 0$, which is is a trivial case.

However, there are pairs of states which are of the same form in Eqs. (3.40)-(3.43) and have the same optimal CHSH operator. The collections of such states pairs are listed as follows

$$\begin{aligned} \Phi \equiv& \{(|\Phi_{(\theta)}\rangle, |\Phi_{(\frac{\pi}{2}-\theta)}\rangle)\}, \\ \Omega \equiv& \{(|\Omega_{(\theta)}\rangle, |\Omega_{(\frac{\pi}{2}-\theta)}\rangle)\}, \\ \Lambda \equiv& \{(|\Lambda_{(\theta,\delta)}\rangle, |\Lambda_{(-\theta,\delta)}\rangle)\}, \\ \Pi \equiv& \{(|\Pi_{(\theta,\delta)}\rangle, |\Pi_{(-\theta,\delta)}\rangle)\}. \end{aligned}$$

Moreover, we could not find out any three two-qubit states which are of the same form and have the same optimal CHSH operator. Thus, at most two different two-qubit pure states could have the same optimal CHSH operator.

Note that any two-qubit pure state can be written as $|\Phi_{(\theta)}\rangle = \cos\theta|00\rangle + \sin\theta|11\rangle$ up to some local unitaries. Applying Lemma 3, we find out that any pair of two-qubit states in the sets Ω, Λ and Π can be transformed into a pair of states in the set Φ via the same local unitary operations. Thus, we only need to consider the pairs of states in the collection Φ in order to figure out all pairs of two-qubit states that have the same optimal CHSH operators. Applying Lemma 2, we find out that the two-qubit pure states $|\Phi_{(\theta)}\rangle$ and $|\Phi_{(\frac{\pi}{2}-\theta)}\rangle$ share the same optimal CHSH operators $S_{\theta+} = \frac{2}{\sqrt{1+\sin^2 2\theta}}(\sin 2\theta\sigma_x \otimes \sigma_x + \sigma_z \otimes \sigma_z)$ and $S_{\theta-} = \frac{2}{\sqrt{1+\sin^2 2\theta}}(-\sin 2\theta\sigma_y \otimes \sigma_y + \sigma_z \otimes \sigma_z)$.

We conclude the above analysis as the following theorem which is the main result of this subsection.

Theorem 2. *Two different two-qubit pure states $|\psi\rangle$ and $|\psi'\rangle$ have the same optimal CHSH operator if and only if they can be written as*

$$
\begin{aligned}
|\psi\rangle &= (U_A \otimes U_B)(\cos\theta|00\rangle + \sin\theta|11\rangle) \text{ and} \\
|\psi'\rangle &= (U_A \otimes U_B)(\sin\theta|00\rangle + \cos\theta|11\rangle),
\end{aligned}
$$

where U_A, U_B are some unitaries on $\mathcal{H}_2$ and $\theta \in [0, \pi)$. The optimal CHSH operators for both $|\psi\rangle$ and $|\psi'\rangle$ are $(U_A \otimes U_B)S_{\theta+}(U_A \otimes U_B)^\dagger$ and $(U_A \otimes U_B)S_{\theta-}(U_A \otimes U_B)^\dagger$ where

$$
\begin{aligned}
S_{\theta+} &= \frac{2}{\sqrt{1+\sin^2 2\theta}}(\sin 2\theta\sigma_x \otimes \sigma_x + \sigma_z \otimes \sigma_z) \text{ and} \\
S_{\theta-} &= \frac{2}{\sqrt{1+\sin^2 2\theta}}(-\sin 2\theta\sigma_y \otimes \sigma_y + \sigma_z \otimes \sigma_z).
\end{aligned}
$$

At most two of two-qubit pure states can have a same optimal CHSH operator.

3.4 The nonlocality is upper bounded by entanglement

In this section, we show that the nonlocality of a general two-qubit state is upper bounded by a function of the corresponding entanglement. We further figure out the class of two-qubit states of which the upper bound of nonlocality can be reached.

According to the Schmidt decomposition [68], any pure state of a two-qubit system can be written as

$$|\Phi_\theta\rangle = \cos\theta|00\rangle + \sin\theta|11\rangle, \theta \in [0, \frac{\pi}{4}], \tag{3.44}$$

upper to some local unitary transformations. As the entanglement and nonlocality are invariant under local unitary transformations, it is sufficient to investigate the state $|\Phi_\theta\rangle$ in order to qualitatively analyze the entanglement and nonlocality of an arbitrary two-qubit pure state.

In the last section, we have figured out that the correlation matrix of the state $|\Phi_\theta\rangle$ is a diagonal matrix with diagonal entries being $\sin 2\theta$, $-\sin 2\theta$ and 1. By applying Lemma 2, it is obvious that the nonlocality of the state $|\Phi_\theta\rangle$ is

$$\mathcal{N}(\Phi_\theta) = 2\sqrt{1 + \sin^2 2\theta}. \tag{3.45}$$

According to the definition in Eq. (3.3), we get the concurrence of the state $|\Phi_\theta\rangle$ as follows

$$C(\Phi_\theta) = |tr(|\Phi_\theta\rangle\langle\Phi_\theta|Y \otimes Y)| = |T_{22}| = |\sin 2\theta|. \tag{3.46}$$

Thus, it is straightforward to get the relationship between the nonlocality and entanglement of a two-qubit pure state. We conclude the above analysis as the following lemma.

Lemma 4. *Suppose $|\psi\rangle$ is an arbitrary pure state of a two-qubit system. The nonlocality and concurrence of $|\psi\rangle$ is related by the following equation*

$$\mathcal{N}(\psi) = 2\sqrt{1 + C(\psi)^2}. \tag{3.47}$$

This simple relationship between the nonlocality and concurrence of a general two-qubit pure state has been mentioned in literatures [82, 83].

Now, we consider the relationship between the nonlocality and entanglement of a general two-qubit state. Inspired by that relationship of an arbitrary pure state, we conjecture that the nonlocality of a mixed two-qubit state is closely related to the function $2\sqrt{1 + C(\rho)}$ of the concurrence $C(\rho)$. Hence, we numerically compare the values $\mathcal{N}(\rho)$ and $2\sqrt{1 + C(\rho)}$ over 5000 randomly generated two-qubit mixed states through computer simulation, which are plotted in Fig. 3.1. Each red point stands for a randomly generated state with the corresponding coordinate being $(C(\rho)$,

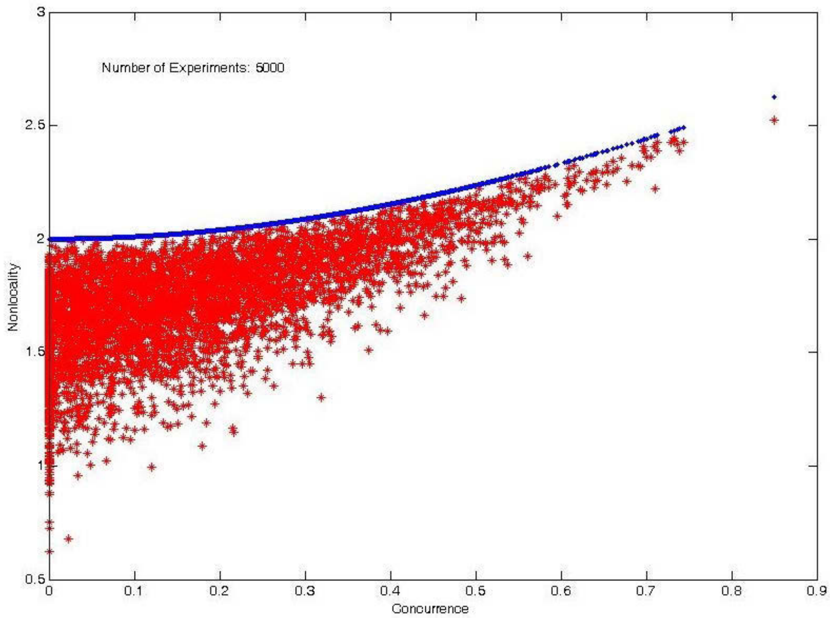

Fig. 3.1: A numerical illustration of the relationship between nonloclaity and concurrence of general two-qubit states.

$\mathcal{N}(\rho)$). The blue points are generated according to the function $2\sqrt{1+C(\rho)}$ of the concurrence $C(\rho)$. Obviously, the nonlocality of a general two-qubit state ρ is upper bounded by the value $2\sqrt{1+C(\rho)}$. When the state is pure, the nonlocality reaches the upper bound, which has been mathematically proved and further concluded in Lemma 4.

We conclude the observation as the following theorem and further give an analytical proof.

Theorem 3. *Suppose ρ is an arbitrary density operator of a two-qubit system with concurrence being C. Then, the nonlocality of ρ is upper bounded by*

$$\mathcal{N}(\rho) \leq 2\sqrt{1+C^2}, \tag{3.48}$$

where the equality holds if and only if $\rho \in \mathcal{Q}$. The set $\mathcal{Q}$ of density operators on $\mathcal{H}_2^{\otimes 2}$ is defined as follows

$$\mathcal{Q} \equiv \{(U_A \otimes U_B)(p|\varphi_1\rangle\langle\varphi_1| + (1-p)|\varphi_2\rangle\langle\varphi_2|)(U_A \otimes U_B)^\dagger\},$$

where U_A, U_B are arbitrary unitaries on $\mathcal{H}_2$, $p \in [0,1]$, $|\varphi_1\rangle = \cos\theta|00\rangle + \sin\theta|11\rangle$ and $|\varphi_2\rangle = \sin\theta|00\rangle + \cos\theta|11\rangle$ for some $\theta \in [0, \pi)$.

Proof. According to Lemma 1, there is a decomposition $\rho = \sum_k p_k |\psi_k\rangle\langle\psi_k|$, where $p_k \geq 0$ and $\sum_k p_k = 1$, such that $C(\psi_k) = C$ for all states $|\psi_k\rangle$. Combining the convexity of nonlocality and Lemma 4, we have

$$\begin{aligned}\mathcal{N}(\rho) &\leq \sum_k p_k \mathcal{N}(\psi_k) \\ &= \sum_k p_k 2\sqrt{1 + C(\psi_k)^2} \\ &= 2\sqrt{1 + C^2}.\end{aligned} \tag{3.49}$$

The equality in Eq. (3.49) holds if and only if the optimal CHSH operator of the state ρ also acts as the optimal CHSH operator for the state $|\psi_k\rangle$ for all k. Namely, all pure states $|\psi_k\rangle$ should have a same optimal CHSH operator in order to achieve the equality. Through the discussion in Section 3.3, we find that at most two different two-qubit pure states could have the same optimal CHSH operator. According to Theorem 2, any two different two-qubit pure states have the same optimal CHSH operator if and only if they can be written as $U_A \otimes U_B(\cos\theta|00\rangle + \sin\theta|11\rangle)$ and $U_A \otimes U_B(\sin\theta|00\rangle + \cos\theta|11\rangle)$ for some local unitary operators U_A and U_B on $\mathcal{H}_2$ and $\theta \in [0, \pi)$. Equivalently, the equality in Eq. (3.49) holds if and only if the state $\rho \in \mathcal{Q}$, namely ρ can be written as a mixture of $|\varphi_1\rangle$ and $|\varphi_2\rangle$ up to some local unitaries.

Therefore, we have

$$\mathcal{N}(\rho) \leq 2\sqrt{1 + C^2}, \tag{3.50}$$

with equality if and only if $\rho \in \mathcal{Q}$. $\square$

4. QUANTIFICATION OF GENUINE TRIPARTITE NONLOCALITY

We have discussed the nonlocality generated from bipartite quantum resources in the last chapter. The definitions and basic results for the nonlocality of bipartite scenario can be extended to that of multipartite scenarios. The simplest multipartite nonlocality test scenario is the one consisted with three participants, which is also known as tripartite nonlocality.

In this chapter, we will exploit the tripartite nonlocality. Our research is mainly focused on the detection and quantification of genuine tripartite nonlocality. The work reported in this chapter is based our publication in *Quantum Information Processing* [84].

4.1 *Definition of tripartite nonlocality*

The nonlocality of tripartite scenario has a more complex structure than that of bipartite scenario, which makes it an interesting but difficult question for understanding. Similarly with the research of bipartite nonlocality, the objects of tripartite nonlocality research are correlations generated from the tripartite nonlocality test scenario. The tripartite nonlocal correlations could be generated from the scenario when resources share between participants are quantum states. The existence of tripartite nonlocality could be sufficiently convinced by the violation of the corresponding Bell inequalities.

In a tripartite nonlocality test scenario, there are three separated participants, say Alice, Bob and Clare. Suppose measurement settings of Alice, Bob and Clare are denoted by x, y and z while the corresponding measurement outcomes are denoted by a, b and c, respectively. The stochastic characteristics of the scenario is completely described by the correlation $p(a, b, c|x, y, z)$.

The tripartite nonlocality has several different definitions. A natural generalization of the basic LHVM, which is defined in Eq. (2.23) for bipartite scenario, to the tripartite scenario is

$$p(a,b,c|x,y,z) = \sum_{\lambda} p(\lambda)p(a|x,\lambda)p(b|y,\lambda)p(c|z,\lambda), \tag{4.1}$$

where λ is the hidden variable shared by the three participants and $p(\lambda)$ is the corresponding probability distribution. Any tripartite correlation that can be decomposed into the form of Eq. (4.1) is local. Otherwise, it is nonlocal. This kind of nonlocality is known as standard tripartite nonlocality. However, this definition is only sufficient to characterize the two-way nonlocality where only two parties share nonlocal resource and they are classically correlated to the third party. For example, the three parties share the correlation $p(a,b,c|x,y,z) = p(a|x)p(b,c|y,z)$ where $p(b,c|y,z)$ is a bipartite nonlocal correlation. Although Alice is not nonlocally correlated to Bob and Clare, the correlation is nonlocal according to the definition in Eq. (4.1).

A kind of more interesting LHVM is the one where some common resources are shared by the three participants. The correlations that do not coincide with this LHVM are a class of more precious nonlocal resource. Thus, this kind of nonlocality is also known as genuine tripartite nonlocality. The first definition of genuine tripartite nonlocality is proposed by Svetlichny in 1987 [52]. According to Svetlichny's definition, a tripartite correlation is local if it admits a LHVM defined as follows:

$$\begin{aligned} p(a,b,c|x,y,z) = &\sum_{\lambda} p(\lambda)p(a|x,\lambda)p(b,c|y,z,\lambda) \\ &+ \sum_{\mu} p(\mu)p(b|y,\mu)p(a,c|x,z,\mu) \\ &+ \sum_{\nu} p(\nu)p(c|z,\nu)p(a,b|x,y,\nu), \end{aligned} \tag{4.2}$$

where λ, μ and ν are shared hidden variables and $\sum_{\lambda} p(\lambda) + \sum_{\mu} p(\mu) + \sum_{\nu} p(\nu) = 1$. This is a convex combination of three terms, in each of which at most two parties are nonlocally correlated. The local correlation defined in Eq. (4.2) is known as S_2 local. A correlation is genuinely nonlocal if it cannot be written as the decomposition of S_2 local definition. This definition of nonlocality prevents the two-way nonlocality. Thus, this kind of nonlocality is also known as genuine tripartite nonlocality or Svetlichny nonlocality.

Definitions of weaker genuine tripartite nonlocality can be given when constraints are added to the bipartite correlation in each term of Svetlichny's LHVM [51]. A correlation of the form of Eq. (4.2) is NS_2 local if the bipartite terms are nonsignaling. Otherwise, it is genuinely three-way NS nonlocal. Correlation of the form of Eq. (4.2) are T_2 local if the time ordering of the measurements are considered. Otherwise, they are said to be genuinely three-way nonlocal. Let T_2, NS_2 and S_2 stand for the set of T_2 local correlations, NS_2 local correlations and S_2 local correlations, respectively. The relationship of the sets is $NS_2 \subset T_2 \subset S_2$ where the inclusion is strict [51].

Detecting and quantifying the tripartite nonlocality are tasks of practical significance. A sufficient condition for detecting the tripartite nonlocality is the violation of the Bell inequalities. And the nonlocality of a tripartite correlation can be quantified by the amount of the maximal violation of the corresponding Bell inequality. Two popular Bell inequalities for the tripartite nonlocality are Mermin inequality [85] and Svetlichny inequality [52]. Any standard tripartite local correlation, defined in Eq. (4.1), satisfies the Mermin inequality. However, there are tripartite correlations which can maximally violate the Mermin inequality but admit the Svetlichny inequality [86]. Namely, the Mermin inequality is not strong enough to detect the genuine tripartite nonlocality. The drawback of Mermin inequality can be made up by the Svetlichny inequality. The tripartite local correlations with perspective to any of the LHVM definitions we have discussed satisfy the Svetlichny inequality. Svetlichny inequality not only can detect the genuinely three-way nonlocality and the genuinely three-way NS nonlocality, but also can detect the Svetlichny's genuine tripartite nonlocality. Therefore, the violation of Svetlichny inequality is a sufficient condition to detect the genuine tripartite nonlocal, which is the strongest form of tripartite nonlocality.

In this chapter, we will concentrate on Svetlichny's definition of tripartite nonlocality, also referred as genuine tripartite nonlocality. Svetlichny inequality is the corresponding Bell inequality for detecting and quantifying the genuine tripartite nonlocality. We will investigate the genuine tripartite nonlocality of a three-qubit system.

4.2 Tripartite nonlocality test scenario and Svetlichny inequality

In this section, we first review the quantum experimental scenario for testing genuine tripartite nonlocality. Then, we introduce a Bell inequality for detecting and quantifying the genuine tripartite nonlocality generated from the scenario, namely Svetlichny inequality.

Suppose that Alice, Bob and Clare are three seperated participants in the tripartite nonlocality test scenario. A joint quantum system consisted of three-qubit is shared by the participants. And each participant owns a single qubit quantum system. Every participant performs a dichotomic projective measurement which is chosen from two possible measurement settings. Recall that any projective measurement on a single qubit system can be described by an observable which is a Hermitian operator with eigenvalues $+1$ and -1. The observable can be equivalently represented as $\vec{r}\cdot\vec{\sigma}$ where $\vec{r}$ is a three dimensional real unit vector and $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is the vector of Pauli matrices. In the following discussion, we denote the elements of a row vector $\vec{r} \in \mathbb{R}^3$ as r_k with $k = 1, 2, 3$, namely $\vec{r} = (r_1, r_2, r_3)$.

Without loss of generality, suppose the two measurement observables for Alice's system are $X = \vec{x}\cdot\vec{\sigma}$ and $X' = \vec{x'}\cdot\vec{\sigma}$ where $\vec{x}$ and $\vec{x'}$ are unit vectors in $\mathbb{R}^3$. Similarly, let $Y = \vec{y}\cdot\vec{\sigma}$ and $Y' = \vec{y'}\cdot\vec{\sigma}$ be measurement observables for Bob's system, and $Z = \vec{z}\cdot\vec{\sigma}$ and $Z' = \vec{z'}\cdot\vec{\sigma}$ be that for Clare's system. Note that $\vec{y}, \vec{y'}, \vec{z}, \vec{z'}$ are all unit vectors in $\mathbb{R}^3$. Suppose ρ is the three-qubit quantum state shared by the three participants. And the outcomes of Alice, Bob and Clare's measurement operations are denoted by a, b and c, respectively. The scenario can be depicted in Figure. 4.1.

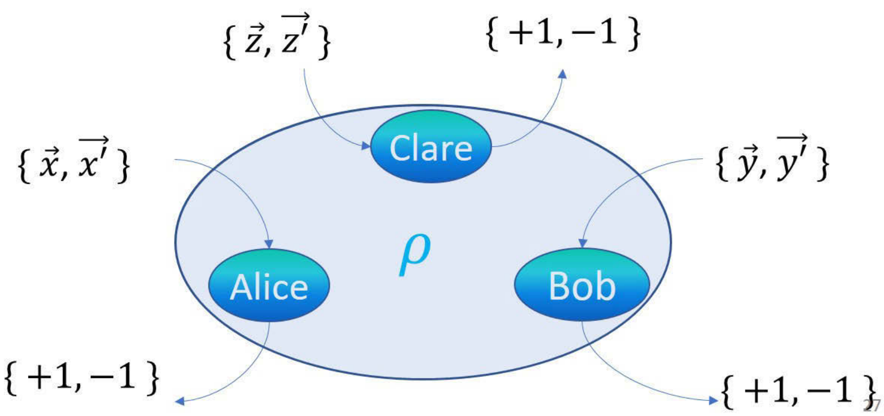

Fig. 4.1: The scenario of testing genuine tripartite nonlocality.

According to the theory of quantum mechanics, a quantum correlation can be generated from the scenario, which is shown as follows:

$$p(a,b,c|x,y,z) = tr((X_a^x \otimes Y_b^y \otimes Z_c^z)\rho), \tag{4.3}$$

where X_a^x is the measurement operator corresponding to the measurement outcome a on condition that Alice chooses the measurement observable X and the similar definitions apply for the measurement operators Y_b^y and Z_c^z.

A quantum state ρ is said to be S_2 local if any correlation generated from the scenario with the state ρ admits the Svetlichny's LHVM defined in Eq. (4.2). Otherwise, the state ρ is said to be genuinely tripartite nonlocal. Any S_2 local quantum state ρ satisfies the Svetlichny inequality

$$tr(S\rho) \leq 4, \tag{4.4}$$

for all possible Svetlichny operators

$$S \equiv (X + X') \otimes (Y \otimes Z' + Y' \otimes Z) + (X - X') \otimes (Y \otimes Z - Y' \otimes Z'). \tag{4.5}$$

Conversely, the violation of this inequality for some Svetlichny operator S is a sufficient evidence that the state is genuinely tripartite nonlocal.

A common choice for quantifying the genuine tripartite nonlocality of a three-qubit state is the maximal violation of the Svetlichny inequality by the state [55]. Let $S(\rho)$ denote the maximal violation of the Svetlichny inequality of the state ρ. Namely,

$$S(\rho) \equiv \max_S tr(S\rho), \tag{4.6}$$

where the maximum is over all possible Svetlichny operators. Then, $S(\rho)$ can be regarded as the quantity of the genuine nonlocality of the state ρ.

A more comprehensive measure for quantifying the genuine tripartite nonlocality can be based on the amount of maximal violation of the Svetlichny inequality. Note that the maximal violation of the Svetlichny inequality over all three-qubit states is $S_{max} = 4\sqrt{2}$ and the maximal violation value can be obtained by setting the GHZ state $|GHZ\rangle = (|000\rangle + |111\rangle)/\sqrt{2}$ as the quantum resource for the genuine tripartite nonlocality test scenario [52]. Thus, we can define a quantity $\mathcal{N}_G(\rho)$ to measure the nonlocality of the state ρ as follows:

$$\mathcal{N}_G(\rho) = \max\left\{0, \frac{S(\rho)-4}{S_{max}-4}\right\}. \tag{4.7}$$

It is obvious that $\mathcal{N}_G(\rho)$ is monotonically increasing and ranges from 0 to 1 as $S(\rho)$ goes from 4 to S_{max}. $\mathcal{N}_G(\rho)$ equals 0 if and only if the Svetlichny inequality of ρ holds for any possible Svetlichny operators while it equals 1 when the violation of Svetlichny inequality reaches the maximal violation value S_{max}. Therefore, $\mathcal{N}_G(\rho)$ is a comprehensive measure of the genuine tripartite nonlocality for a three-qubit state ρ. And $\mathcal{N}_G(\rho) > 0$ is a sufficient condition for the three-qubit state ρ exhibiting genuine tripartite nonlocality.

Note that calculating $S(\rho)$ is a necessary step to get the measure $\mathcal{N}_G(\rho)$ of the genuine tripartite nonlocality of the state ρ. Moreover, the quantity $S(\rho)$ can be viewed as a kind of measure of the genuine tripartite nonlocality of ρ in its own right. Thus, we will concentrate on calculating $S(\rho)$ for quantitatively analyzing the genuine tripartite nonlocality of the state ρ. In the following discussions, we will refer $S(\rho)$ the genuine tripartite nonlocality of the three-qubit state ρ. The term genuine tripartite nonlocality will be interchangeably used in perspectives of qualitative detection and quantitative analysis.

4.3 The genuine nonlocality of general three-qubit states

Recall that any state ρ of a three-qubit system can be expressed in the Pauli basis as follows

$$\rho = \frac{1}{8}\sum_{i,j,k=0}^{3} t_{ijk}\sigma_i \otimes \sigma_j \otimes \sigma_k, \tag{4.8}$$

where $t_{ijk} = tr(\rho\sigma_i \otimes \sigma_j \otimes \sigma_k) \in \mathbb{R}$. Note that the genuine tripartite nonlocality $S(\rho)$ defined in Eq. (4.6) is the maximal value of $tr(S\rho)$ over all possible Svetlichny operators. The quantity $tr(S\rho)$ is composed of 8 terms each of which is an expectation value of the multiplication of the corresponding measurement outcomes. Each term is of the form shown as follows:

$$tr[\rho(X \otimes Y \otimes Z)] = \sum_{i,j,k=1}^{3} x_i y_j z_k t_{ijk} \equiv \langle \vec{x}, T_z \vec{y} \rangle, \tag{4.9}$$

where $T_k = (t_{ijk})$ are 3 by 3 real matrices of Pauli coefficients indexed by i and j for $k = 1, 2, 3$ and T_z is a combination of the matrices T_k with the elements of $\vec{z}$ being the corresponding weights, namely $T_z \equiv \sum_{k=1}^{3} z_k T_k$. Here $\langle \cdot, \cdot \rangle$ denotes the normal inner product in $\mathbb{R}^3$ and we abuse the notation slightly by writing $T_z\vec{y}$ for $T_z\vec{y}^T$.

It is obviously to notice that the genuine nonlocality of a three-qubit state is only related to 27 real numbers, which are elements of Pauli coefficient matrices T_1, T_2 and T_3, out of the 64 Pauli coefficients defined in Eq. (4.8). Those 27 coefficients determine the properties of the connection between the whole three joint particles of the three-qubit system while the others only contain the local information of single-qubit subsystems or two-qubit subsystems. In the following, we refer T_1, T_2 and T_3 the correlation matrices of the three-qubit state ρ. The three correlation matrices can form a cube, denoted by T, which has unique properties with respect to genuine tripartite nonlocality. The cube and correlation matrices can be depicted in Fig. 4.2. Elements of matrix T_1 are represented in the top layer of the correlation cube. That of T_2 and T_3 are represented in the middle and bottom layer, respectively.

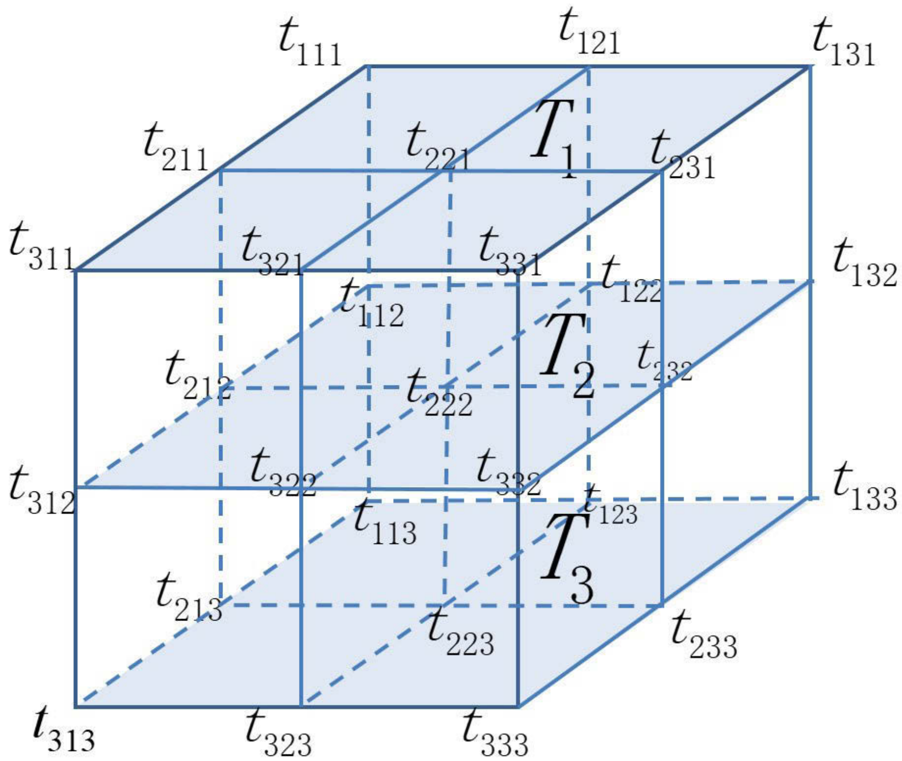

Fig. 4.2: The correlation cube for the genuine nonlocality of a general three-qubit state.

Let $\vec{e_0}$ and $\vec{e_1}$ be two unit vectors such that $\vec{x} + \vec{x'} = 2\cos\alpha\vec{e_0}$ and $\vec{x} - \vec{x'} =$

$2\sin\alpha\vec{e_1}$ for some $\alpha\in[0,\frac{\pi}{2})$. Note that $\vec{e_0}$ and $\vec{e_1}$ are also orthogonal. Let $E\equiv\vec{e_0}\cdot\vec{\sigma}$ and $E'\equiv\vec{e_1}\cdot\vec{\sigma}$. Then, the left side of Svetlichny inequality can be equivalently written as

$$
\begin{aligned}
tr(S\rho)=&2\cos\alpha tr(E\otimes(Y\otimes Z'+Y'\otimes Z))+2\sin\alpha tr(E'\otimes(Y\otimes Z-Y'\otimes Z'))\\
=&2\cos\alpha\langle\vec{e_0},\vec{\lambda_0}\rangle+2\sin\alpha\langle\vec{e_1},\vec{\lambda_1}\rangle,
\end{aligned}
\tag{4.10}
$$

where vectors $\vec{\lambda_0}$ and $\vec{\lambda_1}$ are defined as follows:

$$\vec{\lambda_0}\equiv T_{z'}\vec{y}+T_z\vec{y'}, \tag{4.11}$$

$$\vec{\lambda_1}\equiv T_z\vec{y}-T_{z'}\vec{y'}. \tag{4.12}$$

Applying the Cauchy-Schwarz inequality, we get

$$tr(S\rho)\leq 2\sqrt{\langle\vec{e_0},\vec{\lambda_0}\rangle^2+\langle\vec{e_1},\vec{\lambda_1}\rangle^2}, \tag{4.13}$$

where the equality holds when

$$
\begin{aligned}
\cos\alpha=&\langle\vec{e_0},\vec{\lambda_0}\rangle/\sqrt{\langle\vec{e_0},\vec{\lambda_0}\rangle^2+\langle\vec{e_1},\vec{\lambda_1}\rangle^2} \qquad \text{and}\\
\sin\alpha=&\langle\vec{e_1},\vec{\lambda_1}\rangle/\sqrt{\langle\vec{e_0},\vec{\lambda_0}\rangle^2+\langle\vec{e_1},\vec{\lambda_1}\rangle^2}.
\end{aligned}
$$

To make further optimization, we establish an orthogonal coordinate system along the plane specified by vectors $\vec{\lambda_0}$ and $\vec{\lambda_1}$ with vector $\vec{\lambda_0}$ being one of the axes. Let $\vec{\lambda_0}=(u,0,0)$ and $\vec{\lambda_1}=(v,w,0)$ where $u\equiv\|\vec{\lambda_0}\|$, $v\equiv\langle\vec{\lambda_0},\vec{\lambda_1}\rangle/\|\vec{\lambda_0}\|$ and $w\equiv\sqrt{\|\vec{\lambda_1}\|^2-v^2}$. Suppose $\vec{e_0}=(\sin\theta_0,\cos\theta_0\sin\eta_0,\cos\theta_0\cos\eta_0)$ and $\vec{e_1}=(\sin\theta_1,\cos\theta_1\sin\eta_1,\cos\theta_1\cos\eta_1)$ where parameters $\theta_0,\eta_0,\theta_1,\eta_1\in[0,2\pi)$. Then, it follows that

$$
\begin{aligned}
&\langle\vec{e_0},\vec{\lambda_0}\rangle^2+\langle\vec{e_1},\vec{\lambda_1}\rangle^2\\
=&u^2\sin{\theta_0}^2+(v\sin\theta_1+w\cos\theta_1\sin\eta_1)^2\\
\equiv&g(\theta_0,\eta_0,\theta_1,\eta_1).
\end{aligned}
\tag{4.14}
$$

Now, the problem of calculating the genuine tripartite nonlocality $S(\rho)$ comes to the problem of optimizing the function $g(\theta_0,\eta_0,\theta_1,\eta_1)$ with the constraint shown as follows:

$$\langle\vec{e_0},\vec{e_1}\rangle=\sin\theta_0\sin\theta_1+\cos\theta_0\cos\theta_1\cos(\eta_0-\eta_1)=0.$$

By applying the method of Lagrange multipliers, we find out that the function $g(\theta_0, \eta_0, \theta_1, \eta_1)$ is upper bounded as follows:

$$g(\theta_0, \eta_0, \theta_1, \eta_1) \leq \frac{1}{2}((u^2 + v^2 + w^2) + \sqrt{(u^2 - v^2 + w^2)^2 + 4v^2w^2}), \tag{4.15}$$

where the equality holds when $\eta_0 = \eta_1 = \frac{\pi}{2}$, $\theta_1 = \arccos\sqrt{\frac{1}{2}(1 + \frac{u^2 - v^2 + w^2}{\sqrt{(u^2-v^2+w^2)^2+4v^2w^2}})}$ and $\theta_0 = \theta_1 + \frac{\pi}{2}$. With some simple calculations, we find out that the upper bound can be equivalently written as follows:

$$\langle \vec{e_0}, \vec{\lambda_0} \rangle^2 + \langle \vec{e_1}, \vec{\lambda_1} \rangle^2 \leq \frac{1}{2}((\|\vec{\lambda_0}\|^2 + \|\vec{\lambda_1}\|^2) + \sqrt{(\|\vec{\lambda_0}\|^2 + \|\vec{\lambda_1}\|^2)^2 - 4\langle \vec{\lambda_0}, \vec{\lambda_1} \rangle^2}), \tag{4.16}$$

where the equality can be achieved for properly chosen measurement variables $\vec{x}$ and $\vec{x'}$. In fact, the derivation of the upper bound is the process of optimizing the quantity $\langle \vec{e_0}, \vec{\lambda_0} \rangle^2 + \langle \vec{e_1}, \vec{\lambda_1} \rangle^2$ over the measurement variables $\vec{x}$ and $\vec{x'}$. Note that $\vec{\lambda_0}$ and $\vec{\lambda_1}$ defined in Eqs.(4.11) and (4.12) are combinations of the measurement variables $\vec{y}, \vec{y'}, \vec{z}$, $\vec{z'}$ and the correlation matrices T_1, T_2, T_3 of the state ρ. Let $F(T_1, T_2, T_3)$ represent the maximal value of the quantity $\langle \vec{e_0}, \vec{\lambda_0} \rangle^2 + \langle \vec{e_1}, \vec{\lambda_1} \rangle^2$, which is only related to the correlation matrices of ρ. The calculation of $F(T_1, T_2, T_3)$ is a further optimization over the measurement variables $\vec{y}, \vec{y'}, \vec{z}$ and $\vec{z'}$. Formally, it can be defined as follows

$$F(T_1, T_2, T_3) \equiv \max_{\vec{y}, \vec{y'}, \vec{z}, \vec{z'}} \frac{1}{2}\left(\left(\|\vec{\lambda_0}\|^2 + \|\vec{\lambda_1}\|^2\right) + \sqrt{\left(\|\vec{\lambda_0}\|^2 + \|\vec{\lambda_1}\|^2\right)^2 - 4\langle \vec{\lambda_0}, \vec{\lambda_1} \rangle^2}\right), \tag{4.17}$$

where the maximum is over all possible measurement variables $\vec{y}, \vec{y'}, \vec{z}$ and $\vec{z'}$. Note that $F(T_1, T_2, T_3)$ is a function of the correlation matrices of ρ. Obviously, it follows that

$$tr(S\rho) \leq 2\sqrt{F(T_1, T_2, T_3)}, \tag{4.18}$$

where the equality can be achieved by properly choosing the measurement settings. According to the definition in Eq. (4.6), the right side of the inequality is the genuine tripartite nonlocality of the state ρ. Namely, the genuine nonlocality of the state ρ can be equivalently written as

$$S(\rho) = 2\sqrt{F(T_1, T_2, T_3)}. \tag{4.19}$$

We summarize our main result in this section as the following theorem.

Theorem 4. *Suppose ρ is the density operator of a three-qubit system whose correlation matrices are T_1, T_2 and T_3. Then, the genuine tripartite nonlocality of the state ρ is*

$$S(\rho) = 2\sqrt{F(T_1, T_2, T_3)}, \tag{4.20}$$

where the function F is defined in Eq. (4.17).

4.4 Properties of genuine tripartite nonlocality

In the last section, we have simplified the problem of genuine nonlocality to an optimization problem with fewer free variables. However, it is still not obvious to get an analytical expression of the function in Eq. (4.17). In this section, we will conclude some properties of the genuine nonlocality which can simplify the problem.

Lemma 5. *Let ρ be a three-qubit state with correlation matrices T_1, T_2 and T_3. Then,*

$$S(\rho) \leq \max_{\vec{y},\vec{y'},\vec{z},\vec{z'}} 2\sqrt{\|\vec{\lambda_0}\|^2 + \|\vec{\lambda_1}\|^2} \tag{4.21}$$

where $\vec{\lambda_0}$ and $\vec{\lambda_1}$ are defined in Eqs.(4.11) and (4.12). Furthermore, if the maximum on the right-hand side of Eq. (4.21) can be obtained for some $\vec{\lambda_0}$ and $\vec{\lambda_1}$ with $\vec{\lambda_0} \perp \vec{\lambda_1}$, then the equality holds.

Proof. Applying the Cauchy-Schwartz inequality, we get an inequality as follows:

$$\langle \vec{e_0}, \vec{\lambda_0}\rangle^2 + \langle \vec{e_1}, \vec{\lambda_1}\rangle^2 \leq \|\vec{\lambda_0}\|^2 + \|\vec{\lambda_1}\|^2.$$

The above inequality is an immediate result of the Eq. (4.16). Combining the inequality with the Eq. (4.13), it is obvious that the inequality in Eq. (4.21) is true. Thus, we have proved the upper bound.

Suppose there are unit vectors $\vec{y}$, $\vec{y'}$, $\vec{z}$, and $\vec{z'}$ which achieve the maximum on the right-hand side of Eq. (4.21) and make $\vec{\lambda_0} \perp \vec{\lambda_1}$. Note that the inner product $\langle \vec{\lambda_0}, \vec{\lambda_1}\rangle = 0$. Then, it follows that

$$\begin{aligned}
&\frac{1}{2}\left(\left(\|\vec{\lambda_0}\|^2 + \|\vec{\lambda_1}\|^2\right) + \sqrt{\left(\|\vec{\lambda_0}\|^2 + \|\vec{\lambda_1}\|^2\right)^2 - 4\langle \vec{\lambda_0}, \vec{\lambda_1}\rangle^2}\right) \\
=&\|\vec{\lambda_0}\|^2 + \|\vec{\lambda_1}\|^2 \\
=&F(T_1, T_2, T_3).
\end{aligned}$$

Applying Theorem 4, we get that the equality in Eq. (4.21) holds as follows:

$$S(\rho) = 2\sqrt{F(T_1, T_2, T_3)} = 2\sqrt{\|\vec{\lambda_0}\|^2 + \|\vec{\lambda_1}\|^2}.$$

Therefore, we have proved the lemma. □

The genuine nonlocality of a special class of three-qubit states can be obtained with this lemma. By applying the above lemma, we can get an analytical expression of genuine nonlocality for the generalized GHZ states which coincides with the result obtained by Ghose *et al.* [55]. This result will be illustrated in the next section.

Lemma 6. *Suppose T_1, T_2 and T_3 are correlation matrices of a three-qubit state ρ. If T'_k are correlation matrices of another three-qubit state ρ' such that $T_k = wT'_k, k = 1, 2, 3$ for some parameter $w \in \mathbb{R}$, the genuine nonlocality of ρ is related to that of ρ' by*

$$S(\rho) = |w|S(\rho'). \tag{4.22}$$

Proof. Combining Eqs.(4.9), (4.11) and (4.12), we can know that

$$\vec{\lambda_0} = w\vec{\lambda'_0}, \tag{4.23}$$

$$\vec{\lambda_1} = w\vec{\lambda'_1}, \tag{4.24}$$

where $\vec{\lambda'_0}$ and $\vec{\lambda'_1}$ follow the same definition in Eqs.(4.11) and (4.12) while the correlation matrices T_k are replaced with T'_k. By taking Eqs.(4.23) and (4.24) into Eq. (4.17), we can get

$$F(T_1, T_2, T_3) = |w|^2 F(T'_1, T'_2, T'_3).$$

Then, the result can be easily proved by applying Theorem 4. □

A class of important quantum states of a three-qubit system are the generalized Werner states

$$\rho_{WS} = p|GHZ\rangle_{\pm}\langle GHZ| + (1-p)\frac{I}{8}, \tag{4.25}$$

where $0 \leq p \leq 1$ and $|GHZ\rangle_{\pm} = (|000\rangle \pm |111\rangle)/\sqrt{2}$ are GHZ states. The genuine nonlocality of GHZ states all equal $S_{max} = 4\sqrt{2}$ which is the maximal among the three-qubit states [52]. As an application of Lemma 6, we get that the genuine nonlocality of the three-qubit generalized Werner state is $S(\rho_{WS}) = 4\sqrt{2}p$. And ρ_{WS} is genuinely tripartite nonlocal when $p > \frac{1}{\sqrt{2}}$.

The quantification of the genuine nonlocality of a general three-qubit state is an optimization problem over 6 measurement settings which correspond to 12 free real variables. In the discussions of the last section, we have optimized the problem over the measurement settings of Alice. In fact, we can also start the optimization from other participant. Note that the Svetlichny operator in Eq. (4.5) is symmetric and can be equivalently written as:

$$S = (X \otimes Y + X' \otimes Y') \otimes (Z + Z') + (X \otimes Y' - X' \otimes Y) \otimes (Z - Z'). \tag{4.26}$$

And the basic term of the quantification of genuine tripartite nonlocality, which is shown in Eq. (4.9), is also equivalent to the equation as follows:

$$tr[\rho(X \otimes Y \otimes Z)] = \sum_{i,j,k=1}^{3} x_i y_j z_k t_{ijk} = \langle \vec{z}, R_y \vec{x} \rangle, \tag{4.27}$$

where R_j are 3 by 3 correlation matrices with elements being $(R_j)_{ki} = t_{ijk}$ and the matrix $R_y = \sum_{j=1}^{3} y_j R_j$ is a combination of the correlation matrices with the weights taking values according to the elements in the vector $\vec{y}$. Thus,

$$tr(S\rho) = \langle \vec{z} + \vec{z'}, \vec{\omega_0} \rangle + \langle \vec{z} - \vec{z'}, \vec{\omega_1} \rangle, \tag{4.28}$$

where $\vec{\omega_0} \equiv R_y \vec{x} + R_{y'} \vec{x'}$ and $\vec{\omega_1} \equiv R_{y'} \vec{x} - R_y \vec{x'}$. Note that

$$F(R_1, R_2, R_3) = \max_{\vec{x}, \vec{x'}, \vec{y}, \vec{y'}} \frac{1}{2}((\|\vec{\omega_0}\|^2 + \|\vec{\omega_1}\|^2) + \sqrt{(\|\vec{\omega_0}\|^2 + \|\vec{\omega_1}\|^2)^2 - 4\langle \vec{\omega_0}, \vec{\omega_1} \rangle^2}). \tag{4.29}$$

By applying the same method for the proof of Theorem 4, we find out that the genuine tripartite nonlocality of the three-qubit state ρ can be equivalently written in the form follows:

$$S(\rho) = 2\sqrt{F(R_1, R_2, R_3)}. \tag{4.30}$$

We can also start the optimization of the problem from the measurement settings of Clare's system. Similarly, we can get the genuine tripartite nonlocality of the state ρ as follows:

$$S(\rho) = 2\sqrt{F(Q_1, Q_2, Q_3)}, \tag{4.31}$$

where $Q_i \equiv (t_{ijk})$ for $i = 1, 2, 3$ are 3 by 3 correlation matrices indexed by j and k.

The elements of the correlation matrices R_1, R_2 and R_3 correspond to the left, middle and right layers of correlation cube T in Fig. 4.2, respectively. The correlation matrices Q_1, Q_2 and Q_3 correspond to the back, middle and front layers of the correlation cube, respectively. Hence, the genuine tripartite nonlocality of a three-qubit state has inherent symmetry which can also be concluded in the following lemma.

Lemma 7. *The genuine nonlocality of a three-qubit state ρ is determined by a set of correlation matrices which can be chosen from the corresponding correlation cube through any direction. To be specific,*

$$\begin{aligned} S(\rho) &= 2\sqrt{F(T_1, T_2, T_3)} \\ &= 2\sqrt{F(R_1, R_2, R_3)} \\ &= 2\sqrt{F(Q_1, Q_2, Q_3)}, \end{aligned} \tag{4.32}$$

where $\{T_1, T_2, T_3\}$, $\{R_1, R_2, R_3\}$ and $\{Q_1, Q_2, Q_3\}$ are sets of correlation matrices choosing from the correlation cube through different directions.

4.5 Genuine tripartite nonlocality of special classes of three-qubit states

We have analyzed the genuine tripartite nonlocality of general states of three-qubit system and got an simplified expression of it in Section 4.3. We have also developed some properties for the genuine tripartite nonlocality of general three-qubit states in Section 4.4.

In this section, we apply the theorem and lemmas developed in the previous sections to analyze the genuine tripartite nonlocality of some special classes of three-qubit states. We will discuss the generalized GHZ states in subsection 4.5.1, the GHZ-symmetric states in subsection 4.5.2 and two classes of three-qubit states which have special correlation matrices in subsections 4.5.3 and 4.5.4. Eventually, analytical expressions of the genuine tripartite nonlocality of those states will also be obtained.

4.5.1 The generalized GHZ states

The pure states of a three-qubit system can be genuinely entangled in two different ways, namely GHZ-class states and W-class states [87]. By means of stochastic local operations and classical communication (SLOCC), any entangled three-qubit pure state can be converted into either GHZ state or W state with nonzero probability. An important type of GHZ-class states is the generalized GHZ state shown as follows:

$$|G_\theta\rangle = \cos\theta|000\rangle + \sin\theta|111\rangle.$$

In this subsection, we analyze and further get an analytical expression of the genuine tripartite nonlocality of the generalized GHZ state by applying the results obtained in the previous sections.

Note that the correlation matrices of the generalized GHZ state are $T_k = \sin 2\theta T_k'$, $k=1,2,3$, where

$$T_1' = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad T_2' = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad T_3' = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \cot 2\theta \end{pmatrix}.$$

Suppose T_k' are correlation matrices of a three-qubit state ρ'. Applying the Lemma 6, it is obvious that

$$S(G_\theta) = |\sin 2\theta| S(\rho').$$

Now, it is equivalent to quantify the genuine tripartite nonlocality of the state ρ' to get the genuine tripartite nonlocality of the generalized GHZ state. Suppose $\vec{y} = (\sin\beta\sin\eta, \sin\beta\cos\eta, \cos\beta)$, $\vec{y'} = (\sin\beta'\sin\eta', \sin\beta'\cos\eta', \cos\beta')$, $\vec{z} = (\sin\gamma\sin\varphi, \sin\gamma\cos\varphi, \cos\gamma)$ and $\vec{z'} = (\sin\gamma'\sin\varphi', \sin\gamma'\cos\varphi', \cos\gamma')$. According the definitions in Eqs.(4.11) and (4.12), the vectors $\vec{\lambda_0}$ and $\vec{\lambda_1}$ corresponding to the correlation matrices T_k' are

$$\vec{\lambda_0} = \begin{pmatrix} -\sin\beta'\sin\gamma\cos(\eta'+\varphi) - \sin\beta\sin\gamma'\cos(\eta+\varphi') \\ -\sin\beta'\sin\gamma\sin(\eta'+\varphi) - \sin\beta\sin\gamma'\sin(\eta+\varphi') \\ \cot 2\theta(\cos\beta'\cos\gamma + \cos\beta\cos\gamma') \end{pmatrix},$$

and

$$\vec{\lambda_1} = \begin{pmatrix} -\sin\beta\sin\gamma\cos(\eta+\varphi) + \sin\beta'\sin\gamma'\cos(\eta'+\varphi') \\ -\sin\beta\sin\gamma\sin(\eta+\varphi) + \sin\beta'\sin\gamma'\sin(\eta'+\varphi') \\ \cot 2\theta(\cos\beta\cos\gamma - \cos\beta'\cos\gamma') \end{pmatrix},$$

respectively. We further calculate

$$
\begin{aligned}
& \|\vec{\lambda'_0}\|^2 + \|\vec{\lambda'_1}\|^2 \\
= & \cot^2 2\theta(\cos^2\beta + \cos^2\beta')(\cos^2\gamma + \cos^2\gamma') + 4\sin\beta\sin\beta'\sin\gamma\sin\gamma'\sin(\eta-\eta')\sin(\varphi-\varphi') \\
& + (\sin^2\beta + \sin^2\beta')(\sin^2\gamma + \sin^2\gamma') \\
\leq & \cot^2 2\theta(\cos^2\beta + \cos^2\beta')(\cos^2\gamma + \cos^2\gamma') + 4|\sin\beta\sin\beta'\sin\gamma\sin\gamma'| \\
& + (\sin^2\beta + \sin^2\beta')(\sin^2\gamma + \sin^2\gamma') \\
\leq & \cot^2 2\theta(\cos^2\beta + \cos^2\beta')(\cos^2\gamma + \cos^2\gamma') + 2(\sin^2\beta + \sin^2\beta')(\sin^2\gamma + \sin^2\gamma'),
\end{aligned}
$$

where the last inequality is from the fact that

$$4\sin\beta\sin\beta'\sin\gamma\sin\gamma' \leq (\sin^2\beta + \sin^2\beta')(\sin^2\gamma + \sin^2\gamma'),$$

for any β, β', γ, and γ'. Let $x \equiv \sin^2\beta + \sin^2\beta'$ and $y \equiv \sin^2\gamma + \sin^2\gamma'$. Then,

$$
\begin{aligned}
& \|\vec{\lambda'_0}\|^2 + \|\vec{\lambda'_1}\|^2 \\
& \leq (2 + \cot^2 2\theta)xy - 2\cot^2 2\theta(x+y) + 4\cot^2 2\theta \\
& \equiv f(x,y).
\end{aligned}
$$

Note that the function $f(x,y)$ is symmetric with respect to x and y, and if $x < y$, then $f(x+\epsilon, y-\epsilon) > f(x,y)$ whenever $0 < \epsilon < y - x$. Thus, $f(x,y)$ reaches its maximum at some point with $x = y$. Inserting $x = y$ into the formula, and noting that $x, y \in [0,2]$, we have

$$f(x,y) \leq \begin{cases} 8 & \text{if } \cot^2 2\theta \leq 2 \\ 4\cot^2 2\theta & \text{if } \cot^2 2\theta > 2, \end{cases}$$

where for the above case, the equality holds when $x = y = 2$, while for the below one, it holds when $x = y = 0$.

When $\cot^2 2\theta \leq 2$, a simple calculation shows that the maximum of $\|\vec{\lambda'_0}\|^2 + \|\vec{\lambda'_1}\|^2$ can be achieved by taking $\beta = \beta' = \gamma = \gamma' = \eta = \varphi = \pi/2$ while $\eta' = \varphi' = 0$. In this case, $\vec{\lambda'_0} = (0, -2, 0)$ and $\vec{\lambda'_1} = (2, 0, 0)$. Thus, $\vec{\lambda'_0} \perp \vec{\lambda'_1}$, and by Lemma 5, we derive $S(G_\theta) = 4\sqrt{2}|\sin 2\theta|$.

When $\cot^2 2\theta > 2$, the maximum of $\|\vec{\lambda'_0}\|^2 + \|\vec{\lambda'_1}\|^2$ can be achieved by taking $\beta = \beta' = \gamma = \gamma' = 0$ while other parameters arbitrarily. In this case, $\vec{\lambda'_0} = (0, 0, 2\cot 2\theta)$ and $\vec{\lambda'_1} = (0, 0, 0)$. Thus, $\vec{\lambda'_0} \perp \vec{\lambda'_1}$, and by Lemma 5, we derive $S(G_\theta) = 4|\cos 2\theta|$.

Note that the condition $\cot^2 2\theta > 2$ is equivalent to $\sin^2 2\theta < \frac{1}{3}$. Therefore, the genuine tripartite nonlocality, namely the maximal violation of Svetlichny inequalities, of the generalized GHZ states is

$$S(G_\theta) = \begin{cases} 4|\cos 2\theta| & \text{if } \sin^2 2\theta < \frac{1}{3} \\ 4\sqrt{2}|\sin 2\theta| & \text{if } \sin^2 2\theta \geq \frac{1}{3}, \end{cases}$$

which coincides the result obtained by Ghose *et al.* [55]. The generalized GHZ state $|G_\theta\rangle$ is genuinely tripartite nonlocal when $\sin^2 2\theta > \frac{1}{2}$.

4.5.2 Three-qubit GHZ-symmetric states

GHZ-symmetric states is a class of mixed states which play an important role in quantum information research. Eltschka *et al.* completely characterized the three-qubit GHZ-symmetric states [88]. The three-tangle, a quantitative measure of entanglement for three-qubit state, of three-qubit GHZ-symmetric states has been derived by Siewert *et al.* [89]. In 2016, Paul *et al.* analyzed the nonlocality of three-qubit GHZ-symmetric states [58].

As an application of the techniques developed in the previous sections, we work out the genuine nonlocality of three-qubit GHZ-symmetric states in a dramatically simple way in this subsection.

The three-qubit GHZ-symmetric states can be represented as

$$\rho(p,q) = (\frac{2q}{\sqrt{3}} + p)|GHZ\rangle_+\langle GHZ| + (\frac{2q}{\sqrt{3}} - p)|GHZ\rangle_-\langle GHZ| + (1 - \frac{4q}{\sqrt{3}})\frac{I}{8}, \tag{4.33}$$

where the parameter q ranges in the interval $-\frac{1}{4\sqrt{3}} \leq q \leq \frac{\sqrt{3}}{4}$ and for given q, the parameter p is constrained by $|p| \leq (\frac{\sqrt{3}q}{2} + \frac{1}{8})$. This family of states forms a plain triangle which is depicted in Fig. 4.3. Any point in this triangle represents a three-qubit GHZ-symmetric state, which not only includes GHZ states, but also the generalized Werner states, W states, biseparable states and separable states.

The correlation matrices of the state $\rho(p,q)$ are

$$T_1 = \begin{bmatrix} 2p & 0 & 0 \\ 0 & -2p & 0 \\ 0 & 0 & 0 \end{bmatrix}, T_2 = \begin{bmatrix} 0 & -2p & 0 \\ -2p & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \text{ and } T_3 = 0,$$

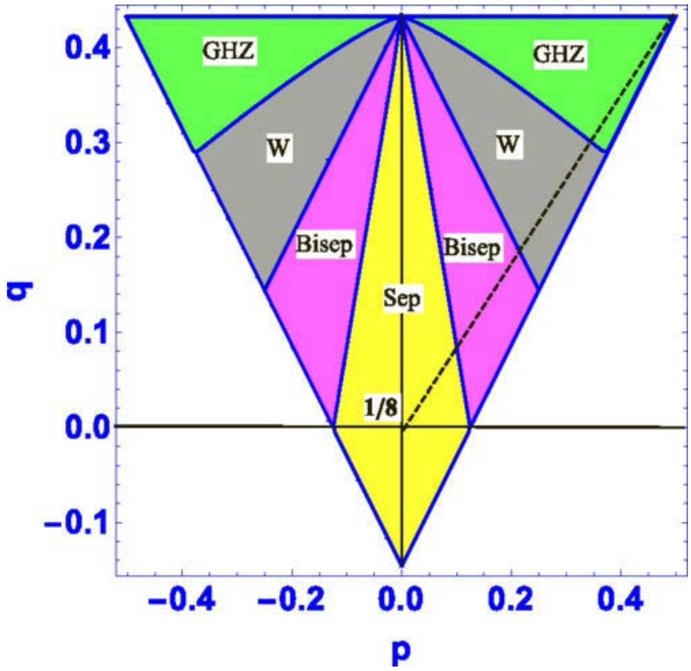

Fig. 4.3: The triangle of GHZ-symmetric states [88, 58].

which can be represented as $T_k = 2pT'_k$ for $k = 1, 2, 3$ and

$$T'_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, T'_2 = \begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \text{ and } T'_3 = 0.$$

It is interesting to note that matrices T'_1, T'_2 and T'_3 are the same with correlation matrices of the GHZ state $|GHZ\rangle_+ = (|000\rangle + |111\rangle)/\sqrt{2}$ of which the genuine tripartite nonlocality achieves the maximum value $S_{max} = 4\sqrt{2}$. Applying Lemma 6, we can get the genuine tripartite nonlocality of the GHZ-symmetric state $\rho(p, q)$ as follows:

$$S(\rho(p, q)) = 8\sqrt{2}|p|. \tag{4.34}$$

Thus, it is trivial to conclude that the three-qubit GHZ-symmetric state $\rho(p, q)$ is genuinely tripartite nonlocal if $|p| > \frac{\sqrt{2}}{4}$. This result is consistent with the one obtained by Paul *et al.* [58].

4.5.3 The state with only one nonzero correlation matrix

In this subsection, we will discuss the genuine tripartite nonlocality of a class of three-qubit states which have only one nonzero correlation matrix.

Suppose ρ is a three-qubit state with correlation matrices T_1, T_2 and T_3. Without loss of generality, let T_1 be the only nonzero correlation matrix, namely $T_2 = T_3 = 0$. Then, the important vectors defined in Eqs. (4.11) and (4.12) can be equivalently written as

$$\begin{aligned}\vec{\lambda_0} &= T_1(z_1'\vec{y} + z_1\vec{y'}) \quad \text{and} \\ \vec{\lambda_1} &= T_1(z_1\vec{y} - z_1'\vec{y'}).\end{aligned}$$

Suppose the real normal matrix $T_1^T T_1$ has a spectral decomposition of the form $T_1^T T_1 = \sum_{k=1}^3 \mu_k \vec{\phi_k}^T \vec{\phi_k}$ where $\{\vec{\phi_1}, \vec{\phi_2}, \vec{\phi_3}\}$ is an orthonormal basis for vector spece $\mathbb{R}^3$ and the corresponding eigenvalues are in nondecreasing order $\mu_1 \geq \mu_2 \geq \mu 3 \geq 0$. With this, we can get the following inequality

$$\begin{aligned}\|\vec{\lambda_0}\|^2 + \|\vec{\lambda_1}\|^2 &= (z_1^2 + {z_1'}^2)(\langle \vec{y}, T_1^T T_1 \vec{y}\rangle + \langle \vec{y'}, T_1^T T_1 \vec{y'}\rangle) \\ &\leq 2 \max_{\vec{y},\vec{y'}}(\langle \vec{y}, T_1^T T_1 \vec{y}\rangle + \langle \vec{y'}, T_1^T T_1 \vec{y'}\rangle) \qquad (4.35) \\ &\leq 4 \max_{\vec{y}} \langle \vec{y}, T_1^T T_1 \vec{y}\rangle \qquad (4.36) \\ &= 4\mu_1,\end{aligned}$$

where the equality in Eq. (4.35) holds when $z_1^2 = {z_1'}^2 = 1$ and the equality in Eq. (4.36) holds when $\vec{y}$, $\vec{y'} \in \{\pm\vec{\phi_1}\}$. Thus, the relationship $\|\vec{\lambda_0}\|^2 + \|\vec{\lambda_1}\|^2 \leq 4\mu_1$ is with equality when both equality in Eqs. (4.35) and (4.36) hold. With some simple calculations, we can find that the inner product $\langle\vec{\lambda_0}, \vec{\lambda_1}\rangle = 0$ when $z_1^2 = {z_1'}^2 = 1$ and $\vec{y}$, $\vec{y'} \in \{\pm\vec{\phi_1}\}$. Applying Lemma 5, we get the genuine tripartite nonlocality $S(\rho) = 4\sqrt{\mu_1}$. The three-qubit state ρ violates the Svetlichny inequality if and only if $\mu_1 > 1$.

We conclude the above discussion as the following theorem.

Theorem 5. *Suppose ρ is a density operator of a three-qubit quantum system with correlation matrices T_1, T_2 and T_3 where $T_2 = T_3 = 0$. Then, the genuine tripartite nonlocality of the state ρ is*

$$S(\rho) = 4\sqrt{\mu_1}, \qquad (4.37)$$

where μ_1 is the largest eigenvalue of the 3 by 3 real normal matrix $T_1^T T_1$. Moreover, the state ρ is genuinely tripartite nonlocal and violates the Svetlichny inequality if $\mu_1 > 1$.

4.5.4 The class of three-qubit states with simultaneously diagonalizable correlation matrices

Theorem 6. *Given ρ is a three-qubit state with simultaneously diagonalizable correlation matrices T_1, T_2 and T_3. Suppose $T_k = \sum_{j=1}^{3} w_{kj} \vec{\psi_j}^T \vec{\psi_j}$, $k = 1, 2, 3$ for an orthonormal basis $\{\vec{\psi_1}, \vec{\psi_2}, \vec{\psi_3}\}$. Then, the genuine tripartite nonlocality of the state ρ is*

$$S(\rho) = 4 \max\{\|\vec{\omega_1}\|, \|\vec{\omega_2}\|, \|\vec{\omega_3}\|\}, \tag{4.38}$$

where vectors $\vec{\omega_j}$ are defined as $\vec{\omega_j} \equiv (w_{1j}, w_{2j}, w_{3j})$ for $j = 1, 2, 3$ and $\|\cdot\|$ stands for the corresponding Euclidean norm. The state ρ is genuinely tripartite nonlocal resource if

$$\max\{\|\vec{\omega_1}\|, \|\vec{\omega_2}\|, \|\vec{\omega_3}\|\} > 1.$$

Proof. We consider the nonlocality test scenario discussed in Section 4.2 and inherit the notations defined in Section 4.3. As the measurement parameters $\vec{y}, \vec{y'}, \vec{z}$ and $\vec{z'}$ are arbitrary unit vectors chosen from the vector space $\mathbb{R}^3$ in this problem, we can assume the vectors are represented in the basis $\{\vec{\psi_j}\}_{j=1}^{3}$. Then, it follows that $T_z\vec{y} = \sum_{k,j=1}^{3} z_k y_j T_k \vec{\psi_j} = \sum_{k,j=1}^{3} z_k y_j \omega_{kj} \vec{\psi_j}$. Note that $\sum_{k,j=1}^{3} z_k \omega_{kj}$ is equal to the inner product $\langle \vec{z}, \vec{\omega_j}\rangle$. Thus, the basic term can be written as $T_z\vec{y} = \sum_{j=1}^{3} y_j \langle \vec{z}, \vec{\omega_j}\rangle \vec{\psi_j}$. The vectors defined in Eqs. (4.11) and (4.12) can be equivalently written as

$$\vec{\lambda_0} = \sum_{j=1}^{3} (y_j \langle \vec{z'}, \vec{\omega_j}\rangle + y'_j \langle \vec{z}, \vec{\omega_j}\rangle)\vec{\psi_j} \quad \text{and}$$
$$\vec{\lambda_1} = \sum_{j=1}^{3} (y_j \langle \vec{z}, \vec{\omega_j}\rangle - y'_j \langle \vec{z'}, \vec{\omega_j}\rangle)\vec{\psi_j}.$$

Further, we get the following inequality

$$\begin{aligned}
\|\vec{\lambda_0}\|^2 + \|\vec{\lambda_1}\|^2 &= \sum_{j=1}^{3} (y_j^2 + {y'_j}^2)(|\langle \vec{z}, \vec{\omega_j}\rangle|^2 + |\langle \vec{z'}, \vec{\omega_j}\rangle|^2) \\
&\leq 2 \max_{\vec{y}, \vec{y'}, \vec{z}} \sum_{j=1}^{3} (y_j^2 + {y'_j}^2) |\langle \vec{z}, \vec{\omega_j}\rangle|^2 \\
&= 4 \max_{\vec{y}, \vec{z}} \sum_{j=1}^{3} y_j^2 |\langle \vec{z}, \vec{\omega_j}\rangle|^2 \\
&= 4 \max\{\|\vec{\omega_1}\|^2, \|\vec{\omega_2}\|^2, \|\vec{\omega_3}\|^2\}.
\end{aligned} \tag{4.39}$$

Without loss of generality, suppose $\|\vec{\omega_1}\|^2$ is the maximal one in the set $\{\|\vec{\omega_1}\|^2, \|\vec{\omega_2}\|^2, \|\vec{\omega_3}\|^2\}$. Namely, $\|\vec{\lambda_0}\|^2 + \|\vec{\lambda_1}\|^2 \leq 4\|\omega_1\|^2$. The equality in Eq. (4.39) holds when $y_1^2 = {y'_1}^2 = 1$, $\vec{z} = \pm\vec{\omega_1}$ and $\vec{z'} = \pm\vec{\omega_1}$. Further, we find out that the inner product $\langle\vec{\lambda_0}, \vec{\lambda_1}\rangle = 0$ when the equality $\|\vec{\lambda_0}\|^2 + \|\vec{\lambda_1}\|^2 = 4\|\omega_1\|^2$ holds. Applying Lemma 5, we get the genuine tripartite nonlocality of the state ρ

$$S(\rho) = 4\|\vec{\omega_1}\|.$$

The state ρ is genuinely tripartite nonlocal if $\|\vec{\omega_1}\|$ is greater than one. Therefore, we have proved the theorem. $\square$

5. DISTRIBUTING NONLOCAL RESOURCE OVER LONG DISTANCE

As the most basic and counterintuitive characteristic of quantum mechanics, quantum nonlocality, a stranger resource than quantum entanglement, plays an indispensable role in most of the quantum information processing applications. Unfortunately, there are insurmountable difficulties in the distribution of quantum resource over remotely located participants.

In this chapter, we concentrate on the problem of distributing nonlocal resources, which include the bipartite nonlocal resources and tripartite genuine nonlocal resources, over distantly separated participants. We propose an effective quantum repeater scheme to distribute bipartite nonlocal quantum resources [90]. We also design a simple protocol to generate the tripartite genuine nonlocal resources from bipartite resources with assistance of LOCC [91].

First, we analyze the challenges in the distribution of quantum resources and then propose possible solutions in Section 5.1. We also review the progresses that have been achieved.

Second, we consider the problem of distributing bipartite nonlocal resources over remotely located participants. We present some basic quantum repeater schemes which consider not only the entanglement-concentration rate but also the LOCC complexity. In Section 5.2, we exploit the basic scenario of quantum repeaters where two different two-qubit pure states are prepared. We construct a protocol which can create maximal entanglement between Alice and Bob at the optimal rate and with less consumption of LOCC resources. A criterion for the projective measurements which are able to achieve the optimal rate of entanglement concentration is prosed in Section 5.3. In Section 5.4, we consider the case in which two general pure states are prepared and general measurements are allowed. We get an upper bound on the probability for a successful measurement operation to produce a maximally entangled state between Alice and Bob.

Last, we consider the problem of distributing genuinely tripartite nonlocal resources over distantly located participants. We propose a simple setting to generate tripartite nonlocality from bipartite resources in Section 5.5. For the scenario, we analyze two classes of bipartite resources, namely two-qubit entangled pure states and Werner states. Upper bounds on the tripartite genuine nonlocality, characterized by the maximal violation of Svetlichny inequalities, are given, and the optimal measurements to achieve these bounds are provided.

The work reported in this chapter is based our publications in *Physical Review A* [92] and *Quantum Information Processing* [91]

5.1 The challenge and solution to the distribution of nonlocal resource

The first step towards the implementation of these applications is to distribute quantum nonlocal resource over remotely located participants. However, there are two basic bottlenecks to directly sending quantum states over a long distance [90]. On one hand, the probability of absorption when transmitting a photon increases exponentially with the distance. For example, a 1-km-long fiber has a transmission of 95%, while the rate for a 1000-km fiber is 10^{-10} Hz, which means that a photon will be transmitted successfully every 300 years [93]. On the other hand, even when a photon arrives at the destination, the fidelity of the transmitted state decreases exponentially with the distance because of the noise in quantum channels. Theoretical results also indicate that it is impossible to find a revised protocol to circumvent this rate-distance trade-off in the application of the quantum key distribution (QKD) [94, 95**?** , 96, 97, 98]. The ultimate limits for the rate-distance trade-off in QKD have been fully established, which include the maximum achievable QKD rate (lower bound) [97] and the tightest upper bound for the rate (upper bound) [98]. For a lossy channel, the upper bound coincides with the lower bound. Thus, this result is the ultimate secret key capacity of a lossy channel, which is also known as PLOB bound.

For the distribution of bipartite quantum resources, an effective solution to overcome the rate-distance trade-off is to use quantum repeaters to divide the long distance into many shorter segments. Each of the segments has a tolerable probability for absorption and noise. In the basic scenario of quantum repeaters, two copies of a bipartite quantum state ρ are shared by three participants, say Alice, Clare, and Bob. Alice and Clare share the copy ρ_{AC}, and Clare and Bob share ρ_{CB}. By performing local operations and classical communication (LOCC) between these three parties, quantum entanglement can be created between Alice and Bob, thereby extending the distance of the entanglement distribution [93]. The basic scenario is depicted in Fig 5.1.

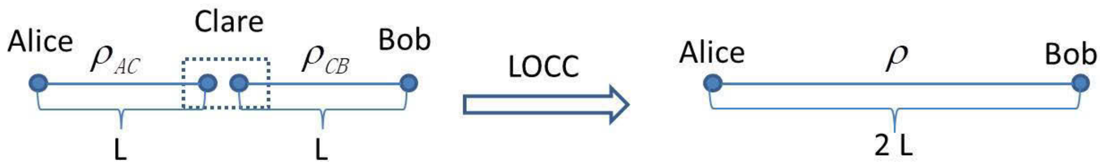

Fig. 5.1: Basic scenario of quantum repeaters.

Since the first protocol was proposed by Briegel in 1998 [90], many schemes for realizing quantum repeaters have been developed [99, 100, 101, 102, 103]. Significant experimental progress has also been made in the last two decades [104, 105, 106, 107, 108, 109]. The performance of quantum repeaters can be assessed by using bounds on the secret-key-agreement capacity of quantum communication channels [? 98].

The basic scenario of quantum repeaters is also known as quantum entanglement swapping [110]. When less entangled pure states are initially distributed in the scenario, the process of concentrating a maximally entangled state is termed entanglement concentration [111, 112]. A simpler scenario is one with only two participants, which has been extensively studied [113, 114, 27, 115]. Many results have also been achieved for quantum entanglement swapping [116, 117, 118, 119, 120]. Bose *et al.* considered the case where the same two-qubit pure states were prepared in each segment [116]. They found the optimal strategy of quantum swapping with respect to concentrating the most entanglement between Alice and Bob. Shi *et al.* considered the case where different two-qubit pure states were prepared [117]. In Shi's strategy, Clare performs a projective measurement in the standard Bell basis.

Then, Alice and Bob perform local operations to create a maximally entangled state between them. Shi *et al.* found out that the optimal entanglement-concentration rate was exactly the same as the concentration rate in the scenario where the less entangled single copy of resource was directly distributed between Alice and Bob. Hardy and Song considered the case where general entangled pure states were distributed in a chain scenario [118]. Perseguers *et al.* exploited the scenario where general two-qubit pure states were distributed in a quantum network [119]. The quantum entanglement swapping configuration can also be used to activate nonlocality from local resources [120].

Beside the essential difficulties in the transmission of quantum resources, there is another important barrier in the distribution of tripartite nonlocality. It is much harder to produce entangled tripartite systems than that of bipartite systems in experimental practice. To overcome this difficulty, Zeilinger et al. [121] proposed a scheme of generating tripartite entanglement from bipartite resources. In the experimental test of nonlocality in GHZ states, the entanglement preparation can also benefit from Zeilinger's scheme [122]. Note that being entangled is the necessary condition of being nonlocal for quantum systems. Therefore, it is a practical solution to distribute genuinely tripartite nonlocal systems via the strategy of generating them from bipartite nonlocal resources.

5.2 *Taking different two-qubit pure states as resource*

In this section, we consider the case where two different pure states of a two-qubit system are prepared in the basic quantum repeater configuration. We construct a protocol to concentrate the maximally entangled two-qubit state between Alice and Bob at the optimal entanglement-concentration rate and with less LOCC complexity. Note that the quantum state of a two-qubit system, which is maximal entangled, is also maximally nonlocal state. Thus, it is identical to distribute quantum resources with respect to maximal entanglement and the maximal nonlocality.

Up to some local unitary operations, any pure state of a two-qubit system can be written as $|\Phi_\theta\rangle \equiv \cos\theta|00\rangle + \sin\theta|11\rangle, \theta \in [0, \frac{\pi}{2}]$. The state $|\Phi_\theta\rangle$ is said to be entangled if $\theta \in (0, \frac{\pi}{2})$. Otherwise, it is separable. When $\theta = \frac{\pi}{4}$, the state is known as the standard maximally entangled state of a two-qubit system, denoted as $|\Phi\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$. Note that quantum entanglement is a kind of resource that cannot be created or increased with LOCC [21]. Particularly, local unitary operations cannot affect the amount of entanglement that exists within entangled quantum systems. Thus, we only need to consider the case where the entangled states $|\Phi_\theta\rangle$ and $|\Phi_\eta\rangle$ with $\theta, \eta \in (0, \frac{\pi}{2})$ are initially distributed in the configuration. A general two-qubit maximally entangled state is equivalent to $|\Phi\rangle$ up to a local unitary operation U, denoted as $|\Phi_U\rangle \equiv (U \otimes I)|\Phi\rangle$. By applying LOCC in the configuration, we expect to obtain a maximally entangled state $|\Phi_U\rangle$ between Alice and Bob such that the rate of entanglement concentration is as high as possible while the LOCC complexity is as low as possible. The configuration is depicted in Fig. 5.2. To achieve this goal, we first need to present some lemmas.

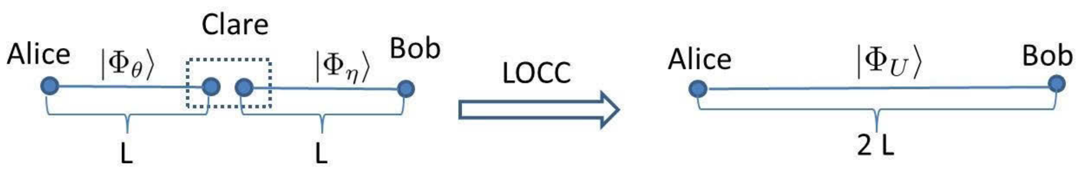

Fig. 5.2: Quantum repeater scheme with different two-qubit pure states.

Lemma 8. *Suppose two parties share a two-qubit state $|\Phi_\lambda\rangle = \cos\lambda|00\rangle + \sin\lambda|11\rangle$ with $\lambda \in (0, \frac{\pi}{2})$. By performing LOCC, the state can be probabilistically transformed into a maximally entangled state. The probability of a successful transformation is upper bounded by $P_E(\Phi_\lambda) \equiv \min\{2\cos^2\lambda, 2\sin^2\lambda\}$.*

Lemma 8, which is an implication of Vidal's result [113], gives the upper bound on the entanglement-concentration rate in the scenario where an entangled two-qubit state $|\Phi_\lambda\rangle$ is shared by two parties. With out loss of generality, suppose $\cos\lambda \geq \sin\lambda$. The upper bound of the concentration rate can be obtained by performing a general measurement $\{M_0, M_1\}$, where $M_0 = \tan\lambda|0\rangle\langle 0| + |1\rangle\langle 1|$ and $M_1 = \sqrt{1-\tan^2\lambda}|0\rangle\langle 0|$, on either party. If the measurement outcome 0 is observed, the maximally entangled state will be created between them. The corresponding probability is $P_E(\Phi_\lambda) = 2\sin^2\lambda$.

Applying Lemma 8, we get the upper bound on the entanglement-concentration rate for the simplest quantum repeater scenario depicted in Fig. 5.2. The result is concluded in the following lemma.

Lemma 9. *Suppose that the two-qubit states* $|\Phi_\theta\rangle$ *and* $|\Phi_\eta\rangle$ *are initially distributed in the scenario depicted in Fig. 5.2. Let* P_{MS} *be the optimal probability that the maximally entangled state can be created between Alice and Bob by applying LOCC. Then,* $P_{MS} \leq \min\{P_E(\Phi_\theta), P_E(\Phi_\eta)\}$.

Proof. We prove this lemma via deducing contradictions. Suppose $P_{MS} > P_E(\Phi_\theta)$. Then, consider a scenario where the resource $|\Phi_\theta\rangle$ is shared by Alice and Bob. Let Bob locally prepare an ancilla state $|\Phi_\eta\rangle$. According to the definition, the probability of creating maximally entangled state between Alice and Bob by applying LOCC is P_{MS}, which is greater than $P_E(\Phi_\theta)$. This result contradicts Lemma 8. Thus, the assumption is not true. It should have $P_{MS} \leq P_E(\Phi_\theta)$. Similarly, we can get $P_{MS} \leq P_E(\Phi_\eta)$.

Therefore, we have $P_{MS} \leq \min\{P_E(\Phi_\theta), P_E(\Phi_\eta)\}$. □

In our protocol, we consider a projective measurement on Clare's joint system. Note that a projective measurement on a two-qubit system consist of four projections. A successful projection of Clare is one where the maximally entangled state can be directly created between Alice and Bob without any further local operations. Our strategy is to construct a projective measurement such that the sum of the probabilities of the successful projections is as high as possible. For projections that result in Alice and Bob sharing non-maximally entangled states, we can apply the probabilistic entanglement concentration by performing a local measurement operation on either Alice's or Bob's system. In general, we can concentrate entanglement from the scenario at a high rate while less of the LOCC resource is consumed.

In the following lemma, we work out the lower and upper bounds on the probability of a successful projection.

Lemma 10. *Assume that the two-qubit pure states* $|\Phi_\theta\rangle$ *and* $|\Phi_\eta\rangle$ *are initially distributed in the scenario shown in Fig. 5.2. Without loss of generality, suppose* $\theta, \eta \in (0, \frac{\pi}{4}]$. *A maximally entangled state can be created between Alice and Bob by projecting Clare's joint system onto state* $|\varphi\rangle$ *without any further local operations. The probability* $p(\varphi)$ *of the successful projection is bounded by*

$$\frac{\sin^2 2\theta \sin^2 2\eta}{4(1+\cos 2\theta \cos 2\eta)} \leq p(\varphi) \leq \frac{\sin^2 2\theta \sin^2 2\eta}{4(1-\cos 2\theta \cos 2\eta)}. \tag{5.1}$$

Proof. The initial state of the three participants' joint quantum system can be written as

$$|\phi_0\rangle_{ABC} = \sum_{k=0}^{3} f_k|k\rangle_{AB}|k\rangle_C, \tag{5.2}$$

where $f_0 = \cos\theta\cos\eta$, $f_1 = \cos\theta\sin\eta$, $f_2 = \sin\theta\cos\eta$ and $f_3 = \sin\theta\sin\eta$. Suppose $|\varphi\rangle = \sum_{k=0}^{3}\mu_k|k\rangle \in \mathcal{H}_2^{\otimes 2}$ with the constraint $\sum_{k=0}^{3}|\mu_k|^2 = 1$. Once the projection occurred, the state of Alice and Bob's joint system would be

$$|\phi\rangle_{AB} = \frac{1}{\sqrt{p(\varphi)}}\langle\phi_C|\phi_0\rangle_{ABC} = \frac{1}{\sqrt{p(\varphi)}}\sum_{k=0}^{3} f_k\mu_k^*|k\rangle_{AB}.$$

As we expect that a maximally entangled state would be created between Alice and Bob without any further local operations, it should have

$$|\phi\rangle_{AB} = (U\otimes I)|\Phi\rangle, \tag{5.3}$$

where U is a unitary operator on $\mathcal{H}_2$.

Let $\Delta_k \equiv \langle k|(U\otimes I)|\Phi\rangle$. Then, the parameters of the projection state and the corresponding probability are related by the formula as follows:

$$f_k\mu_k^* = \sqrt{p(\varphi)}\Delta_k. \tag{5.4}$$

By applying the unit constraint of the projection state $|\varphi\rangle$, we get the probability of the successful projection as follows:

$$p(\varphi) = \left(\sum_{k=0}^{3}\frac{|\Delta_k|^2}{f_k^2}\right)^{-1}. \tag{5.5}$$

Without loss of generality, let $U = |0\rangle\langle\alpha_0| + |1\rangle\langle\alpha_1|$, where $|\alpha_0\rangle = e^{i\tau_0}(\cos\alpha|0\rangle + e^{i\gamma}\sin\alpha|1\rangle)$ and $|\alpha_1\rangle = e^{i\tau_1}(\sin\alpha|0\rangle - e^{i\gamma}\cos\alpha|1\rangle)$ with $\alpha,\tau_0,\tau_1,\gamma \in [0,2\pi)$. It is trivial to determine that $|\Delta_0|^2 = |\Delta_3|^2 = \frac{1}{2}\cos^2\alpha$ and $|\Delta_1|^2 = |\Delta_2|^2 = \frac{1}{2}\sin^2\alpha$. Hence, any successful projection state $|\varphi\rangle$ should be equivalently written as

$$|\varphi\rangle = \sqrt{\frac{p(\varphi)}{2}}(\cos\alpha(\frac{1}{f_0}|00\rangle + e^{i\beta}\frac{1}{f_3}|11\rangle) + e^{i\beta'}\sin\alpha(\frac{1}{f_1}|01\rangle + e^{i\beta''}\frac{1}{f_2}|10\rangle)), \tag{5.6}$$

where $\alpha,\beta,\beta',\beta'' \in [0,2\pi)$. The inverse of the probability can be rewritten as

$$p(\varphi)^{-1} = \frac{1}{2}(\frac{1}{f_1^2} + \frac{1}{f_2^2}) + \frac{1}{2}\cos^2\alpha(\frac{1}{f_0^2} + \frac{1}{f_3^2} - \frac{1}{f_1^2} - \frac{1}{f_2^2}).$$

As we have assumed that $\theta, \eta \in (0, \frac{\pi}{4}]$, it follows that

$$\frac{1}{f_0^2} + \frac{1}{f_3^2} - \frac{1}{f_1^2} - \frac{1}{f_2^2} = \frac{16\cos 2\theta \cos 2\eta}{\sin^2 2\theta \sin^2 2\eta} \geq 0.$$

Hence, the inverse of the successful projection probability $p(\varphi)^{-1}$ reaches the maximum when $\cos^2\alpha = 1$ while it reaches the minimum when $\cos^2\alpha = 0$. Namely,

$$p(\varphi)^{-1} \leq \frac{1}{2}(\frac{1}{f_0^2} + \frac{1}{f_3^2}) = \frac{4(1+\cos 2\theta \cos 2\eta)}{\sin^2 2\theta \sin^2 2\eta}, \tag{5.7}$$

and

$$p(\varphi)^{-1} \geq \frac{1}{2}(\frac{1}{f_1^2} + \frac{1}{f_2^2}) = \frac{4(1-\cos 2\theta \cos 2\eta)}{\sin^2 2\theta \sin^2 2\eta}. \tag{5.8}$$

Then, Eq. (5.1) follows Eqs. (5.7) and (5.8) immediately. Therefore, we have proved the lemma. □

Suppose Clare performs a projective measurement in the orthonormal basis $\{|\varphi_k\rangle\}_{k=1}^4$ with $p(\varphi_k)$ being the probability of projecting the system into state $|\varphi_k\rangle$ and $|\phi_k\rangle_{AB}$ being the corresponding post-measurement state of Alice and Bob's joint system.

First, let $|\varphi_1\rangle$ be the successful projection such that $p(\varphi_1)$ reaches the upper bound of the projection probability in Eq. (5.1). The condition of achieving the upper bound probability is $\cos\alpha = 0$ in Eq. (5.6). Thus, the projection state can be written as

$$|\varphi_1\rangle = (f_2|01\rangle + e^{i\beta_1} f_1|10\rangle)/\sqrt{f_1^2 + f_2^2}, \tag{5.9}$$

for an arbitrary phase $\beta_1 \in [0, 2\pi)$. The corresponding projection probability is $p(\varphi_1) = \frac{\sin^2 2\theta \sin^2 2\eta}{4(1-\cos 2\theta \cos 2\eta)}$.

Second, we try to construct another successful projection with the corresponding projection state $|\varphi_2\rangle$. The state $|\varphi_2\rangle$ should be of the form of Eq. (5.6). The orthogonality of the projection states $|\varphi_2\rangle$ and $|\varphi_1\rangle$ requires that $\langle\varphi_1|\varphi_2\rangle = 0$, which is equivalent to the following constraint:

$$\sqrt{\frac{p(\varphi)}{2(f_1^2 + f_2^2)}} e^{i\beta'} \sin\alpha \Big(\frac{f_2}{f_1} + e^{i(\beta''-\beta_1)}\frac{f_1}{f_2}\Big) = 0.$$

To let the above constraint hold for general resources $|\Phi_\theta\rangle$ and $|\Phi_\eta\rangle$, it should have $\sin\alpha = 0$. Thus, we get the second projection state as

$$|\varphi_2\rangle = (f_3|00\rangle + e^{i\beta_2} f_0|11\rangle)/\sqrt{f_0^2 + f_3^2}, \tag{5.10}$$

where $\beta_2 \in [0, 2\pi)$ is an arbitrary phase. The corresponding probability of the successful projection is $p(\varphi_2) = \frac{\sin^2 2\theta \sin^2 2\eta}{4(1+\cos 2\theta \cos 2\eta)}$, which is exactly the lower bound of the successful probability.

A simple calculation shows that there is not a third projection state which is of the form of Eq. (5.6) and orthogonal to the projection states $|\varphi_1\rangle$ and $|\varphi_2\rangle$. The other projection states can be chosen as

$$|\varphi_3\rangle = (f_1|01\rangle - e^{i\beta_1} f_2|10\rangle)/\sqrt{f_1^2 + f_2^2}, \tag{5.11}$$

$$|\varphi_4\rangle = (f_0|00\rangle - e^{i\beta_2} f_3|11\rangle)/\sqrt{f_0^2 + f_3^2}, \tag{5.12}$$

with the projection probabilities being $p(\varphi_3) = \frac{f_1^4+f_2^4}{f_1^2+f_2^2}$ and $p(\varphi_4) = \frac{f_0^4+f_3^4}{f_0^2+f_3^2}$, respectively. The corresponding post-measurement states of Alice and Bob's joint system are

$$|\phi_3\rangle_{AB} = (f_1^2|01\rangle - e^{-i\beta_1} f_2^2|10\rangle)/\sqrt{f_1^4 + f_2^4}, \tag{5.13}$$

$$|\phi_4\rangle_{AB} = (f_0^2|00\rangle - e^{-i\beta_2} f_3^2|11\rangle)/\sqrt{f_0^4 + f_3^4}. \tag{5.14}$$

We have figured out a projective measurement for Clare. Two of the projections would directly leave Alice and Bob's joint system in maximally entangled states, while the others would leave them in less entangled states. When the measurement outcome $|\varphi_3\rangle$ or $|\varphi_4\rangle$ is observed, we can still concentrate some entanglement from the less entangled state $|\phi_3\rangle$ or $|\phi_4\rangle$ by performing local operations on either Alice's or Bob's system.

Let q and q' be the probabilities that we can concentrate the maximally entangled state from $|\phi_3\rangle$ and $|\phi_4\rangle$ by performing the corresponding general measurement on Bob's qubit, respectively. As we have assumed that $\theta, \eta \in (0, \frac{\pi}{4}]$, it follows that $f_0 \geq f_3$. With out loss of generality, we suppose $\eta \geq \theta$, which implies that $f_1 \geq f_2$. Applying Lemma 8, we get

$$q = \frac{2f_2^4}{f_1^4 + f_2^4}, q' = \frac{2f_3^4}{f_0^4 + f_3^4}.$$

In general, the maximally entangled resource can be created between Alice and Bob with probability

$$P_{MS} = p(\varphi_1) + p(\varphi_2) + p(\varphi_3)q + p(\varphi_4)q' = 2\sin^2\theta.$$

Note that $2\sin^2\theta$ also equals the optimal probability $P_E(\Phi_\theta)$ that the maximally entangled state can be concentrated in the scenario where the resource $|\Phi_\theta\rangle$ is directly prepared between Alice and Bob. Thus, we have $P_{MS} = P_E(\Phi_\theta)$.

Similarly, we get $P_{MS} = P_E(\Phi_\eta)$ for the case $\theta \geq \eta$. Thus, the maximally entangled resource can be concentrated from the scenario in Fig. 5.2 with probability $P_{MS} = \min\{P_E(\Phi_\theta), P_E(\Phi_\eta)\}$. According to Lemma 9, $P_{MS} \leq \min\{P_E(\Phi_\theta), P_E(\Phi_\eta)\}$. Therefore, the entanglement-concentration rate obtained in our protocol is the optimal one for the scenario.

Upon performing the projective measurement on Clare's joint system, no further local operation is needed when any of the two successful projections is observed. Maximally entangled resources will be directly created between Alice and Bob with probability $\frac{\sin^2 2\theta \sin^2 2\eta}{2(1-\cos^2 2\theta\cos^2 2\eta)}$. Assume that the classical communication channel is liable. It is possible to establish an efficient classical communication agreement for telling Bob to take the corresponding action, namely performs the corresponding local measurement or does not take any action.

Therefore, we have constructed a protocol for extending the distance of the entanglement distribution, which is optimal with respect to the entanglement-concentration rate and efficient in perspective LOCC complexity. With this, we have proved the following theorem, which is the main result of this section.

Theorem 7. *Considering a quantum repeater scheme with different two-qubit pure states $|\Phi_\theta\rangle$ and $|\Phi_\eta\rangle$, the protocol we develop in this section is optimal for perspectives of entanglement-concentration rate, which is $P_{MS} = \min\{P_E(\Phi_\theta), P_E(\Phi_\eta)\}$, and efficient for perspectives of LOCC complexity.*

5.3 Criterion for optimal projective measurements with respect to the entanglement-concentration rate

For the scenario depicted in Fig. 5.2, the projective measurement in the standard Bell basis is also able to achieve the optimal entanglement-concentration rate [117]. Thus, the optimal projective measurement for Clare's joint system is not unique with respect to the entanglement-concentration rate. However, not all projective measurements can achieve that goal. For example, it is impossible to obtain entanglement between Alice and Bob by projecting Clare's system onto separable states.

Hence, it is a practical problem to verify whether a projective measurements is able to concentrate entanglement from the scenario with the optimal rate. The following theorem gives a criterion for such measurements.

Theorem 8. *Suppose two-qubit states $|\Phi_\theta\rangle$ and $|\Phi_\eta\rangle$ with $\theta, \eta \in (0, \frac{\pi}{4}]$ and $\theta \leq \eta$ are initially prepared in the quantum repeater scenario (Fig. 5.2). Considering a projective measurement $\{P_k\}_{k=1}^4$ in our protocol, it is able to achieve the optimal entanglement-concentration rate if and only if*

$$\sum_{k=1}^{4} \sqrt{(tr(T_1 \otimes T_2 P_k))^2 + \sin^2 2\theta |tr(|0\rangle\langle 1| \otimes T_2 P_k)|^2} = \cos 2\theta, \tag{5.15}$$

where $T_1 = \cos^2\theta|0\rangle\langle 0| - \sin^2\theta|1\rangle\langle 1|$ and $T_2 = \cos^2\eta|0\rangle\langle 0| + \sin^2\eta|1\rangle\langle 1|$.

Proof. Suppose $P_k = |\varphi_k\rangle\langle\varphi_k|$ where $\{|\varphi_k\rangle\}_{k=1}^4$ is an orthonormal basis of the space $\mathcal{H}_2^{\otimes 2}$. Note that the initial state of the configuration is $|\Phi_\theta, \Phi_\eta\rangle = \sum_{t=0}^3 f_t |t\rangle_C |t\rangle_{AB}$. In the case that the measurement outcome k is observed, the post-measurement state of Alice and Bob's joint system will be

$$|\phi_k\rangle_{AB} = \frac{1}{\sqrt{p_k}} \sum_{t=0}^{3} f_t \langle\varphi_k|t\rangle |t\rangle_{AB},$$

where p_k is the probability of observing the measurement result k. From Lemma 8, the probability $P_E(\phi_k)$ is twice the square of the state's minimal Schmidt number. It is also equal to twice the minimal eigenvalue of the density operator of either Alice's or Bob's system. On the condition that Alice and Bob share the state $|\phi_k\rangle_{AB}$, the density operator of Alice's system is

$$\rho_A^k \equiv tr_B(|\phi_k\rangle_{AB}\langle\phi_k|) = \frac{1}{p_k} \sum_{t_1,t_2=0}^{1} a_{t_1 t_2}^k |t_1\rangle\langle t_2|,$$

where $a_{t_1 t_2}^k = \theta_{t_1}\theta_{t_2} tr((|t_1\rangle\langle t_2| \otimes T_2)P_k)$. For the purpose of convenience, we take the notation $\theta_0 \equiv \cos\theta$ and $\theta_1 \equiv \sin\theta$. The eigenvalues of ρ_A^k are

$$\lambda_\pm^k = \frac{1}{2p_k}((a_{00}^k + a_{11}^k) \pm \sqrt{(a_{00}^k - a_{11}^k)^2 + 4a_{01}^k a_{10}^k}).$$

As $\lambda_+^k \geq \lambda_-^k$, we get $P_E(\phi_k) = 2\lambda_-^k$.

When all the measurement outcomes are considered, the maximally entangled state can be concentrated from the scenario at rate

$$\begin{aligned} p_s &\equiv \sum_{k=1}^{4} p_k \cdot P_E(\phi_k) \\ &= \sum_{k=1}^{4} ((a_{00}^k + a_{11}^k) - \sqrt{(a_{00}^k - a_{11}^k)^2 + 4a_{01}^k a_{10}^k}). \end{aligned}$$

Note that $\sum_{k=1}^4 a_{00}^k = \sum_{k=1}^4 \cos^2\theta tr((|0\rangle\langle 0| \otimes T_2)P_k) = \cos^2\theta$. Similarly, we get $\sum_{k=1}^4 a_{11}^k = \sin^2\theta$. It is also trivial to see that $a_{00}^k - a_{11}^k = tr((T_1 \otimes T_2)P_k)$ and $4a_{01}^k a_{10}^k = \sin^2 2\theta |tr((|0\rangle\langle 1| \otimes T_2)P_k)|^2$. Thus, the rate p_s can be equivalently written as

$$p_s = 1 - \sum_{k=1}^{4} \sqrt{(tr((T_1 \otimes T_2)P_k))^2 + \sin^2 2\theta |tr((|0\rangle\langle 1| \otimes T_2)P_k)|^2}.$$

According to Theorem 7, the optimal entanglement-concentration rate of the scenario shown in Fig. 5.2 is $2\sin^2\theta$. Therefore, the projective measurement P is able to achieve the optimal entanglement-concentration rate, which means $p_s = 2\sin^2\theta$, if and only if

$$\sum_{k=1}^{4} \sqrt{(tr(T_1 \otimes T_2 P_k))^2 + \sin^2 2\theta |tr(|0\rangle\langle 1| \otimes T_2 P_k)|^2} = \cos 2\theta.$$

□

Simple calculations show that both the projective measurement in the standard Bell basis and the one we proposed in this section fulfill the criterion.

5.4 *The upper bound for the scenario with different general pure states*

In this section, we consider a more general scenario in which different general pure states are prepared and general measurements are allowed. Suppose a general bipartite pure state $|\psi_{AB}\rangle$ is shared by Alice and Clare while $|\psi_{CB}\rangle$ is shared by Clare and Bob. We analyze the measurement outcome which leaves Alice and Bob in a maximally entangled state without any further local operations. We refer to this measurement outcome as a successful measurement outcome. The scenario is depicted in Fig. 5.3. Note that an arbitrary maximally entangled state can be written as $|\Omega_U\rangle \equiv (U \otimes I)|\Omega\rangle$, where U is a local unitary on $\mathcal{H}_d$ and $|\Omega\rangle = \frac{1}{\sqrt{d}}\sum_{k=1}^{d}|k\rangle|k\rangle$ is the standard maximally entangled state.

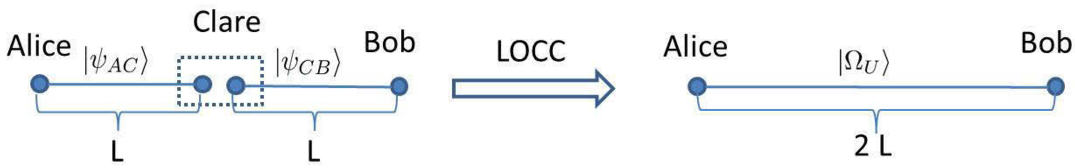

Fig. 5.3: Quantum repeater scenario with two general pure states.

The probability of observing a successful measurement outcome varies for different U's. Theorem 9 gives an upper bound on the probability, which is the main result in this section. To prove Theorem 9, we need two lemmas. Lemma 11 is concluded from Wolf's lecture notes [123]. Lemma 12 is a generalization of a mathematical theorem which has been proved by Lewis [124]. We denote $\lambda_\downarrow(A)$ for the column vector of operator A's eigenvalues in nonincreasing order and $\lambda_\uparrow(A)$ for that in nondecreasing order.

Lemma 11. *Suppose $|\psi\rangle$ is a bipartite pure state of the joint quantum system $A\otimes B$. Let $\rho_A \equiv tr_B(|\psi\rangle\langle\psi|)$ be the density operator of subsystem A. Suppose ρ_A can be expressed as a convex combination $\rho_A = \sum_i \lambda_i \rho_i$, where $\lambda_i > 0$, $\sum_i \lambda_i = 1$ and ρ_i are density operators on $\mathcal{H}_A$. Then, there is a quantum measurement operation on system B, say $T = \{T_i : \mathcal{B}(\mathcal{H}_\mathcal{B}) \to \mathcal{B}(\mathcal{H}_\mathcal{B})\}$, such that*

$$\lambda_i \rho_i = tr_B[(I \otimes T_i)(|\psi\rangle\langle\psi|)]. \tag{5.16}$$

The parameter λ_i can be interpreted as the probability of observing measurement outcome i. The upper bound of λ_i is as follows:

$$\lambda_i \leq \| \rho^{-\frac{1}{2}} \rho_i \rho^{-\frac{1}{2}} \|_\infty^{-1} . \tag{5.17}$$

Lemma 12. *For Hermitian operators A and B,*

$$tr(AB) \geq \lambda_\uparrow(A)^T \lambda_\downarrow(B), \tag{5.18}$$

with equality if and only if there is a unitary operator U such that $U^\dagger AU = diag(\lambda_\uparrow(A))$ and $U^\dagger BU = diag(\lambda_\downarrow(B))$.

Theorem 9. *Suppose the scenario in Fig. 5.3 is prepared with general pure states $|\psi_{AC}\rangle = \sum_{k=1}^{d_A} \sqrt{a_k}|k\rangle|k\rangle$ and $|\psi_{CB}\rangle = \sum_{k=1}^{d_B} \sqrt{b_k}|k\rangle|k\rangle$ where $a_1 \geq \cdots \geq a_{d_A} > 0$, $b_1 \geq \cdots \geq b_{d_B} > 0$ and $d \equiv d_B \geq d_A$. Consider a general measurement $\{M_i\}$ on Clare's joint system. Suppose Alice and Bob will share a maximally entangled state $|\Omega_U\rangle \in \mathcal{H}_d^{\otimes 2}$ after the measurement outcome i is observed by Clare. The corresponding probability p_i of observing measurement outcome i is bounded by*

$$p_i \leq \frac{d}{\sum_{k=1}^{d_A} \frac{1}{a_k b_{d_A+1-k}}} \equiv p_{max}. \tag{5.19}$$

The upper bound probability p_{max} can be achieved if $M_i = \sqrt{p_{max}}|\Omega_U\rangle\langle\Omega_U|\rho_{AB}^{-\frac{1}{2}}$ where $U = \sum_{k=1}^{d_A} |d_A + 1 - k\rangle\langle k| + \sum_{k=d_A+1}^{d} |k\rangle\langle k|$ and ρ_{AB} is the initial state of the Alice and Bob's joint system.

Proof. Initially, Alice and Bob's joint system is in state $\rho_{AB} = \rho_A \otimes \rho_B$ where $\rho_A = \sum_{k=1}^{d} a_k|k\rangle\langle k|$ and $\rho_B = \sum_{k=1}^{d} b_k|k\rangle\langle k|$. Note that we extend ρ_A into the space $\mathcal{H}_d$ by setting $a_k = 0$ for $k > d_A$. In the following discussion, we denote $a_k^{-1} = 0$ for k such that $a_k = 0$.

According to Lemma 11, the probability p_i is upper bounded by

$$p_i \leq \| \rho_{AB}^{-\frac{1}{2}}\rho_U\rho_{AB}^{-\frac{1}{2}} \|_\infty^{-1}, \tag{5.20}$$

where the inverse operator is defined on the corresponding support space. The equality in Eq. (5.20) holds when $M_i^T = \sqrt{p_i}\rho_{AB}^{-\frac{1}{2}}\rho_U$. A simple calculation shows that $\rho_{AB}^{-\frac{1}{2}}|\Omega_U\rangle = \frac{1}{\sqrt{d}}\sum_{k,t=1}^{d} a_k^{-\frac{1}{2}} b_t^{-\frac{1}{2}} \langle k|U|t\rangle|k\rangle|t\rangle$. Thus, we get

$$\begin{aligned}
\|\rho_{AB}^{-\frac{1}{2}}\rho_U\rho_{AB}^{-\frac{1}{2}}\|_\infty =&\|\rho_{AB}^{-\frac{1}{2}}|\Omega_U\rangle\|^2 \\
=&\frac{1}{d}\sum_{k,t=1}^{d} a_k^{-1}b_t^{-1}\langle k|U|t\rangle\langle t|U^\dagger|k\rangle \\
=&\frac{1}{d}tr(U\rho_B^{-1}U^\dagger\rho_A^{-1}).
\end{aligned} \tag{5.21}$$

The eigenvalues of ρ_A^{-1} are $a_{d_A}^{-1} \geq \cdots \geq a_1^{-1} > a_{d_A+1}^{-1} = \cdots = a_d^{-1} = 0$. Those of $U\rho_B^{-1}U^\dagger$ are $b_d^{-1} \geq \cdots \geq b_1^{-1} > 0$. Applying Lemma 12, we get

$$tr(U\rho_B^{-1}U^\dagger\rho_A^{-1}) \geq \sum_{k=1}^{d_A} \frac{1}{a_k b_{d_A+1-k}},$$

where the equality holds when

$$U = \Big(\sum_{k=1}^{d_A} |d_A + 1 - k\rangle\langle k|\Big) \oplus I, \tag{5.22}$$

where the term in the direct sum acts in the kernel space of ρ_A.

Therefore, we get the upper bound of the probability p_i as

$$p_i \leq \frac{d}{\sum_{k=1}^{d_A} \frac{1}{a_k b_{d_A+1-k}}}, \tag{5.23}$$

where the equality holds when the measurement operator is $M_i = \sqrt{p_{max}}|\Omega_U\rangle\langle\Omega_U|\rho_{AB}^{-\frac{1}{2}}$ and U takes the form defined in Eq. (5.22). □

5.5 Generating genuine tripartite nonlocality from bipartite resource

In this section, we analyze the distribution of genuinely tripartite nonlocal resources. Recall that it is difficult to directly produce genuinely tripartite nonlocal resources in experiment. Even if the resource is locally produced, there are essential difficulties to overcome in transmission. However, we have analyzed the distribution of bipartitely nonlocal resources via the scheme of quantum repeaters in last section. Thus, we propose a simple but practical setting, which is shown in Fig. 5.4, for generating genuine tripartite nonlocality from bipartite nonlocal resources.

Suppose there are three remotely located participants Alice, Bob, and Clare. Alice and Bob each shares a copy of the two-qubit nonlocal resource ρ with Clare, denoted as ρ_{AC_1} and ρ_{BC_2}, respectively. Clare then applies a CNOT operation on C_1 (the control qubit) and C_2 (the target qubit) and measures the system C_2 with some projective measurement. Finally, the genuine tripartite nonlocality can be generated between the remaining quantum systems ABC_1 with some probability, which is quantified by the maximal violation of Svetlichny inequalities.

In the following subsections, two different types of resource states are investigated: two-qubit Werner states

$$\rho_W = p|\Phi\rangle\langle\Phi| + (1-p)\frac{I}{4}, \tag{5.24}$$

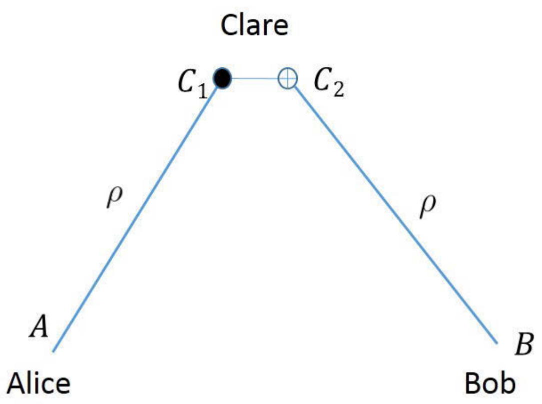

Fig. 5.4: Setting for tripartite nonlocality generation.

where $0 < p < 1$ and $|\Phi\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$, and arbitrarily entangled two-qubit pure states with the Schmidt decomposition

$$|\Phi_\theta\rangle = \cos\theta|00\rangle + \sin\theta|11\rangle, \tag{5.25}$$

where $0 < \theta < \frac{\pi}{2}$.

5.5.1 *Werner states as the resource*

Werner states are an important class of quantum states which show that, rather surprisingly, not all entangled states are nonlocal. This indicates that entanglement and nonlocality are different resources. In this subsection, we consider two-qubit Werner states as the resource in our setting and analyze the nonlocality of post-measurement states.

Suppose the projective measurement applied by Clare on system C_2 is in the following orthonormal basis

$$\begin{aligned} |\psi_0\rangle &= \sin\tau|0\rangle + \cos\tau|1\rangle, & (5.26)\\ |\psi_1\rangle &= \cos\tau|0\rangle - \sin\tau|1\rangle. & (5.27) \end{aligned}$$

If the system is projected to $|\psi_0\rangle$, the post-measurement state of ABC_1 will be

$$\rho_0 = 2\ tr_{C_2}(\rho|\psi_0\rangle\langle\psi_0|),$$

where $\rho = \mathrm{CNOT}_{C_1C_2}(\rho_W \otimes \rho_W)$. The correlation matrices of ρ_0 are $p^2 T_k$, $k = 1, 2, 3$, where

$$T_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & \sin 2\tau \end{pmatrix}, \; T_2 = \begin{pmatrix} 0 & \cos 2\tau & 0 \\ \cos 2\tau & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

and $T_3 = 0$.

We admit the measurement settings for the genuine tripartite nonlocality test scenario which is defined in Section 4. Let $\vec{\lambda_0}$ and $\vec{\lambda_1}$ be the vector variables of the correlation matrices T_k and the measurement vectors according to the definitions in Eqs. (4.11) and (4.12). A routine calculation shows that

$$\begin{aligned}
&\|\vec{\lambda_0}\|^2 + \|\vec{\lambda_1}\|^2 \\
=&\cos^2 2\tau(y_1^2 + y_2^2 + {y_1'}^2 + {y_2'}^2)(z_1^2 + z_2^2 + {z_1'}^2 + {z_2'}^2) \\
&+ 2\sin^2 2\tau(z_1^2 + {z_1'}^2) + 4\cos 2\tau(y_1' y_2 - b_1 y_2')(z_1 z_2' - z_1' z_2).
\end{aligned}$$

Note that the above formula is a homogeneous polynomial of degree 2, and it does not depend on y_3, y_3', z_3, and z_3'. Thus, the maximum of the formula must be obtained at some point where $y_3 = y_3' = z_3 = z_3' = 0$. Then,

$$\max_{\vec{y},\vec{y}',\vec{z},\vec{z}'} (\|\vec{\lambda_0}\|^2 + \|\vec{\lambda_1}\|^2) = 4\cos^2 2\tau + 2 \max_{\vec{y},\vec{y}',\vec{z},\vec{z}'} F(\vec{\lambda_0}, \vec{\lambda_1}),$$

where

$$F(\vec{\lambda_0}, \vec{\lambda_1}) \equiv \sin^2 2\tau(z_1^2 + {z_1'}^2) + 2\cos 2\tau(y_1' y_2 - y_1 y_2')(z_1 z_2' - z_1' z_2).$$

To further optimize $F(\vec{\lambda_0}, \vec{\lambda_1})$, we need the following lemma.

Lemma 13. *For any $u, w \geq 0$ and $\alpha, \beta \in \mathbb{R}$,*

$$u(\cos^2\alpha - \sin^2\beta) + w\sin(\alpha - \beta) \leq \sqrt{u^2 + w^2},$$

and the equality holds if and only if $|\cos 2\alpha| = \frac{u}{\sqrt{u^2+w^2}}$ and $\alpha + \beta = k\pi$ for some integer k.

Proof. Note that

$$\cos^2\alpha - \sin^2\beta = \cos(\alpha+\beta)\cos(\alpha-\beta).$$

The result is then easy from the Cauchy-Schwarz inequality. □

Let $z_1 = \cos\alpha$, $z_2 = \sin\alpha$, $z_1' = \cos\beta$, and $z_2' = \sin\beta$. Then,

$$
\begin{aligned}
&F(\vec{\lambda_0}, \vec{\lambda_1}) \\
&\leq \sin^2 2\tau(\cos^2\alpha + \cos^2\beta) + 2|\cos 2\tau| \cdot |\sin(\alpha-\beta)| \\
&\leq \sin^2 2\tau + \sqrt{\sin^4 2\tau + 4\cos^2 2\tau} \\
&= 2,
\end{aligned}
$$

where the first equality is from the fact that $b_1'b_2 - b_1b_2' \leq 1$ which is in turn from the Cauchy-Schwarz inequality, and the second equality comes from Lemma 13. Furthermore, it is easy to check that the upper bound can be achieved by taking, say,

$$
\begin{aligned}
z_1 = z_1' &= \frac{1}{\sqrt{1+\cos^2 2\tau}}, \\
-z_2 = z_2' &= \frac{\cos 2\tau}{\sqrt{1+\cos^2 2\tau}}, \\
y_1 = -y_2' &= 1, \\
y_2 = y_1' &= 0.
\end{aligned}
$$

In this case, we have

$$
\vec{\lambda_0} = \sqrt{1+\cos^2 2\tau}\ (1,1,0), \quad \vec{\lambda_1} = \sqrt{1+\cos^2 2\tau}\ (1,-1,0).
$$

Thus, $\vec{\lambda_0} \perp \vec{\lambda_1}$, and by Lemma 5,

$$
S(\rho_0) = 4p^2\sqrt{1+\cos^2 2\tau}.
$$

By a similar calculation, we can show that $S(\rho_1) = 4p^2\sqrt{1+\cos^2 2\tau}$ as well, where ρ_1 is the post-measurement state of the joint system ABC_1 when the system C_2 is projected to $|\psi_1\rangle$.

If we choose $\cos\tau = 0$ or $\cos\tau = \pm 1$, which corresponds to the projective measurement in the standard basis on system C_2, the maximal value $4p^2\sqrt{2}$ is achieved for both ρ_0 and ρ_1.

With this, we have proved the following theorem which is the main result of this subsection.

Theorem 10. *Let ρ in Fig. 5.4 be a Werner state defined in Eq. (5.24), and Clare is only allowed to perform projective measurement in the $X-Z$ plane. Then, the* *maximal Svetlichny inequality violation of the remaining states satisfies*

$$p_0 S(\rho_0) + p_1 S(\rho_1) \leq 4p^2\sqrt{2},$$

where ρ_0 and ρ_1 are the post-measurement states of system ABC_1 with the corresponding probabilities p_0 and p_1, respectively. The equality holds when the measurement in the standard basis $\{|0\rangle, |1\rangle\}$ is applied. Furthermore, in this case the maximal violation $4p^2\sqrt{2}$ is achieved for both measurement outcomes; thus, tripartite nonlocality is generated with certainty *if $p > 2^{-\frac{1}{4}} \approx 0.8409$.*

5.5.2 Two-qubit pure states as the resource

Now we turn to the case where an arbitrary two-qubit pure state $|\Phi_\theta\rangle$ described in Eq. (5.25) serves as the resource in our setting. By applying the CNOT operation, the initial state $|\Phi_\theta\rangle_{AC_1}|\Phi_\theta\rangle_{BC_2}$ will be transformed to

$$\begin{aligned}
&|\psi\rangle_{ABC_1C_2} \\
=&\cos^2\theta|0000\rangle + \sin^2\theta|1110\rangle + \sin\theta\cos\theta(|0101\rangle + |1011\rangle) \\
\equiv& h_0|\Phi_0\rangle|0\rangle + h_1|\Phi_1\rangle|1\rangle,
\end{aligned}$$

where $h_0 = \sqrt{\cos^4\theta + \sin^4\theta}$, $h_1 = \sqrt{2}\cos\theta\sin\theta$, and

$$|\Phi_0\rangle = \alpha_0|000\rangle + \alpha_1|111\rangle, \tag{5.28}$$

$$|\Phi_1\rangle = (|010\rangle + |101\rangle)/\sqrt{2}, \tag{5.29}$$

with $\alpha_0 = \frac{\cos^2\theta}{x_0}$ and $\alpha_1 = \frac{\sin^2\theta}{x_0}$.

Suppose Clare measures the system C_2 according to the following orthonormal basis

$$\begin{aligned}
|\varphi_0\rangle &= \mu_0|0\rangle + \mu_1|1\rangle, \\
|\varphi_1\rangle &= \mu_1|0\rangle - \mu_0|1\rangle,
\end{aligned}$$

where $\mu_0, \mu_1 \in \mathbb{R}$ and $\mu_0^2 + \mu_1^2 = 1$. The probability of projecting system C_2 into the state $|\varphi_0\rangle$ is $p_0 = \mu_0^2 h_0^2 + \mu_1^2 h_1^2$, and the post-measurement state of system ABC_1 is

$$|\Psi_0\rangle = (\mu_0 h_0|\Phi_0\rangle + \mu_1 h_1|\Phi_1\rangle)/\sqrt{p_0}. \tag{5.30}$$

The measurement projects system C_2 into $|\varphi_1\rangle$ with probability $p_1 = 1 - p_0$ and the state of ABC_1 becomes

$$|\Psi_1\rangle = (\mu_1 h_0|\Phi_0\rangle - \mu_0 h_1|\Phi_1\rangle)/\sqrt{p_1}. \tag{5.31}$$

To evaluate the nonlocality of the states in Eqs.(5.30) and (5.31), we need a lemma.

Lemma 14. *Let $|\Psi\rangle_{ABC} \equiv \omega_0|\Phi_0\rangle + \omega_1|\Phi_1\rangle$ where $|\Phi_0\rangle$ and $|\Phi_1\rangle$ are defined in Eqs.(5.28) and (5.29) respectively, $\omega_0, \omega_1 \in \mathbb{R}$, and $\omega_0^2 + \omega_1^2 = 1$. Then,*

$$S(\Psi) \leq 4\sqrt{2 + 4\alpha_0\alpha_1(1 + 2\alpha_0\alpha_1)(\omega_0^4 - \frac{1}{2\alpha_0\alpha_1}\omega_0^2)},$$

and the equality holds when

$$12\left(\omega_0^2\alpha_0\alpha_1 - \frac{\omega_1^2}{2}\right)^2 + 2\omega_0^2\omega_1^2(\alpha_0 + \alpha_1)^2 \geq 1. \tag{5.32}$$

Proof. By reordering the systems ABC, the state $|\Psi\rangle$ can be rewritten as

$$|\Psi\rangle_{ACB} = |00\rangle\left(\omega_0\alpha_0|0\rangle + \frac{\omega_1}{\sqrt{2}}|1\rangle\right) + |11\rangle\left(\frac{\omega_1}{\sqrt{2}}|0\rangle + \omega_0\alpha_1|1\rangle\right).$$

Let

$$U = \frac{\omega_0\alpha_0}{\sqrt{r}}\sigma_3 + \frac{\omega_1}{\sqrt{2r}}\sigma_1,$$

be a unitary operator, where σ_1 and σ_3 are Pauli matrices and $r = \omega_0^2\alpha_0^2 + \frac{\omega_1^2}{2}$. Then,

$$(I_{AC} \otimes U_B)|\Psi\rangle_{ACB} = \sqrt{r}|00\rangle|0\rangle + \sqrt{1-r}|11\rangle|\phi\rangle,$$

where

$$|\phi\rangle = \frac{\sqrt{2}\omega_0\omega_1(\alpha_0 + \alpha_1)|0\rangle + (\omega_1^2 - 2\omega_0^2\alpha_0\alpha_1)|1\rangle}{2\sqrt{r(1-r)}}.$$

Note that local unitary operations do not affect nonlocality. Then, the lemma holds from [56]. □

With Lemma 14, we calculate the quadratic mean[1] of the genuine tripartite

[1] For technical reasons, here we consider the quadratic mean, instead of the arithmetic mean as for the Werner states case, to quantify the tripartite nonlocality of the remaining states.

nonlocality as

$$
\begin{aligned}
&\sqrt{p_0 S(\Psi_0)^2 + p_1 S(\Psi_1)^2} \\
&\leq 4\sqrt{2 + 4\alpha_0\alpha_1(2\alpha_0\alpha_1 + 1)\left(h_0^4\left(\frac{\mu_0^4}{p_0} + \frac{\mu_1^4}{p_1}\right) - \frac{h_0^2}{2\alpha_0\alpha_1}\right)} \\
&\leq 4\sqrt{2 + 2(4\alpha_0^2\alpha_1^2 - 1)h_0^2} \\
&= 4\sqrt{\frac{2\sin^2 2\theta}{1 + \cos^2 2\theta}},
\end{aligned}
$$

where the second inequality comes from the fact that

$$\frac{\mu_0^4}{p_0} + \frac{\mu_1^4}{p_1} = \frac{1}{h_0^2}\left(\frac{\mu_0^2}{1 + (\frac{\mu_1 h_1}{\mu_0 h_0})^2} + \frac{\mu_1^2}{1 + (\frac{\mu_0 h_1}{\mu_1 h_0})^2}\right) \leq \frac{1}{h_0^2}(\mu_0^2 + \mu_1^2) = \frac{1}{h_0^2}.$$

The equality holds when $\mu_0^2 = 0$ or $\mu_0^2 = 1$, which correspond to the projective measurement in the standard basis $\{|0\rangle, |1\rangle\}$. In this case, the post-measurement states $|\Psi_0\rangle$ and $|\Psi_1\rangle$ are exactly $|\Phi_0\rangle$ and $|\Phi_1\rangle$ defined in Eqs.(5.28) and (5.29), respectively. If $0.4911 \approx \sqrt{\frac{1}{2} - \frac{1}{2}\sqrt{2 - \sqrt{3}}} \leq \cos\theta \leq \sqrt{\frac{1}{2} + \frac{1}{2}\sqrt{2 - \sqrt{3}}} \approx 0.8711$, then Eq. (5.32) holds for both $|\Psi_0\rangle$ and $|\Psi_1\rangle$, and the upper bound $4\sqrt{\frac{2\sin^2 2\theta}{1+\cos^2 2\theta}}$ is obtained.

We summarize our main result in this subsection as the following theorem.

Theorem 11. *Let $\rho = |\Phi_\theta\rangle\langle\Phi_\theta|$ in Fig. 5.4 where $|\Phi_\theta\rangle$ is defined in Eq. (5.25) with $0.4911 \leq \cos\theta \leq 0.8711$, and Clare is only allowed to perform projective measurement in the $X - Z$ plane. Then, the quadratic mean of the maximal Svetlichny inequality violations of the remaining states satisfies*

$$\sqrt{p_0 S(\Psi_0)^2 + p_1 S(\Psi_1)^2} \leq 4\sqrt{\frac{2\sin^2 2\theta}{1 + \cos^2 2\theta}},$$

where $|\Psi_0\rangle$ and $|\Psi_1\rangle$ are the post-measurement states of system ABC_1 with the corresponding probabilities p_0 and p_1, respectively. The equality holds when the measurement in the standard basis $\{|0\rangle, |1\rangle\}$ is applied. Furthermore, in this case we have $S(\Psi_1) = 4\sqrt{2}$ and

$$S(\Psi_0) = \frac{4\sqrt{2}\sin^2 2\theta}{1 + \cos^2 2\theta}. \tag{5.33}$$

Thus, tripartite nonlocality is generated with certainty *if*

$$0.5412 \approx \sqrt{\frac{2 - \sqrt{2}}{2}} < \cos\theta < \sqrt{\frac{\sqrt{2}}{2}} \approx 0.8409.$$

6. CONCLUSION

Nonlocality, the fundamental feature of quantum mechanics, has been extensively studied since Bell's groundbreaking observation in 1964. As an important application of quantum mechanics, quantum information and quantum computation is a promising interdiscipline and becomes a frontier science. Many protocols of quantum information tasks have significant advantages over their classical counterparts. The core reason behind those advantages is the nonlocality of quantum mechanics. In this dissertation, we have studied problems related to the nonlocality of quantum mechanics in perspectives of both fundamental theory of quantum nonlocality and its applications in quantum information science.

6.1 Conclusion and discussion

The problems studied in this dissertation include the quantitative relationship between entanglement and nonlocality, the quantification of genuine tripartite nonlocality and the distribution of nonlocal quantum resources.

In Chapter 3, we have researched the problem of the same quantum measurement setting for different two-qubit states in perspective of nonlocality test and exploited the quantitative relationship between the entanglement and nonlocality of general two-qubit states. For the former problem, we firstly found the condition that two different general two-qubit states could have the same optimal nonlocality test setting. Then, we found out that at most two different two-qubit pure states could have the same optimal nonlocality test setting and figured out the class of such state pairs. For the later problem, we found out that the amount of nonlocality is upper bounded by a function of the entanglement. Based on the research of the first problem, we analytically proved the fact and found the class of two-qubit states of which the nonlocality could reach the upper bound.

The above results have practical significance. More efficient quantum information processing protocols could be designed by considering the quantum resources of which the nonlocality feature could be optimally stimulated by a same nonlocality test setting. In one situation, we only know the amount of entanglement of a given two-qubit resource while no knowledge about the structure of the state is known. Thus, it is difficult to get the quantity of the nonlocality. By applying the relationship of the nonlocality and entanglement we find in this dissertation, one would be able to know an upper bound for the nonlocality of the state without nonlocality test experiments.

In Chapter 4, we made progress in the quantification of genuine nonlocality of a general three-qubit state which is measured by the maximal violation of Svetlichny inequality. The quantity is related to 27 real numbers among the 64 Pauli coefficients of the state. The quantification of the genuine nonlocality is an optimization problem over 12 free variables. We firstly reduced the problem into another optimization problem over 8 free variables and got a simplified formula. We developed three properties for the genuine nonlocality which could help us to analyze the nonlocality of complex states and understand the nature of quantum nonlocality. Applying the properties, we got analytical results for the genuine nonlocality of five classes of three-qubit states, which include the generalized GHZ states, generalized Werner states, GHZ-symmetric states and two classes of three-qubit states which have special correlation matrices. Note that the genuine nonlocality of generalized GHZ states and GHZ-symmetric states are firstly solved by Ghose *et al.* [55] and Paul *et al.* [58], respectively. They could be easily worked out by applying the strategy and properties developed in the dissertation.

In Chapter 5, we have considered problems in the distributions of quantum nonlocal resources. We have prosed efficient quantum repeater schemes and a new scenario to realize the distribution of bipartite and tripartite quantum systems, respectively.

To distribute the bipartite quantum resources, we designed an quantum repeater scheme, which was efficient with respects to both entanglement-concentration rate and LOCC complexity, to extend the distance of quantum resources distribution. For the scenario with two different two-qubit pure states, we have constructed a protocol to concentrate entanglement. The protocol is optimal for the perspective entanglement-concentration rate and efficient for the perspective LOCC complexity. Further, we found a criterion for the projective measurement to achieve the optimal entanglement-concentration rate. We also examined the scenario where general pure states were prepared and general measurements were allowed. We have got the upper bound on the probability of a successful measurement outcome which produces a maximally entangled state between participants without any further local operations.

The protocol is composed of two steps. First, Clare performs a measurement operation. Second, based on Clare's measurement outcome, Bob chooses the corresponding strategy; namely, Bob does not do any further local operations or performs the corresponding general measurements. In general, the protocol can concentrate entanglement from the scenario with the optimal rate. We reduced the LOCC complexity via the strategy that no further local operation was needed if a maximally entangled state could be created between Alice and Bob when a measurement outcome was observed by Clare.

For the scenario with different two-qubit states $|\Phi_\theta\rangle$ and $|\Phi_\eta\rangle$, we have constructed a projective measurement such that the maximally entangled state could be created after two of the four measurement outcomes. Such measurement outcomes could be observed with probability $\frac{\sin^2 2\theta \sin^2 2\eta}{2(1-\cos^2 2\theta \cos^2 2\eta)}$. If the states for the scenario are the same, say $|\Phi_\theta\rangle$, we can construct a projective measurement with three successful projections to produce maximally entangled states without any further local operations. The corresponding probability is $\frac{\sin^2 2\theta(3+\cos^2 2\theta)}{4(1+\cos^2 2\theta)}$.

To distribute the tripartite nonlocal resources, we have proposed a simple scenario to generate tripartite nonlocal quantum states from bipartite nonlocal resources. We analyzed the cases where Werner states and general pure states of two-qubit system were prepared in the scenario. We found upper bounds the amount of genuine tripartite nonlocality that could be generated from the different resources. We also provided the measurement settings to achieve the upper bounds, respectively. Interestingly, we found that projective measurement according to the standard basis $\{|0\rangle, |1\rangle\}$ achieves the maximal Svetlichny inequality violation of the remaining states in both cases.

6.2 Open questions

A number of questions are raised in the composition of this dissertation. Specifically,

Question 1′. *A more close quantitative relationship between the entanglement and the nonlocality of an arbitrary two-qubit quantum system.*

In this dissertation, we found that the nonlocality of a two-qubit system is upper bound by the entanglement of the state. It is naturally to ask the question whether we can find a more close relation between them. Any breakthrough on this problem would have great significance with respects to both fundamental research of quantum mechanics and the application of quantum information processing tasks.

Question 2′. *Quantitatively analyze the genuine tripartite nonlocality of more complex and important three-qubit states.*

The dissertation provide a new methodology to quantitatively analyze the genuine tripartite nonlocality of three-qubit quantum systems. For future work, we are going to further exploit the power of the strategy and properties we proposed. It is possible that the genuine nonlocality of more complex and important three-qubit states could be analyzed by applying the results. To find an analytical expression of the genuine nonlocality for a general three-qubit state is the interest of our research.

Question 3′. *Design efficient quantum repeater schemes to distribute quantum nonlocality from general quantum resources.*

In this dissertation, we have proposed a quantum repeater scheme to distribute bipartite nonlocality from general two-qubit pure states. We also got partial result for the case of general bipartite pure states.

However, quantum transmission channel would cause noise to quantum systems in experimental practice. It is of practical significance to consider similar quantum repeater scheme but with mixed quantum states being resources. We plan to start with the case of two-qubit mixed states. Then, we will consider quantum system of higher dimension.

Question 4′. *Inspired the efficient quantum repeater, can we find an efficient teleportation protocol?*

In the ordinary sense, teleportation is a scheme that transmits an unknown quantum system from Alice to Bob by preshared entanglement and LOCC. We set a scenario where Clare shares entangled resources with Alice and Bob, respectively. The task is that Alice need to send an unknown quantum system to Bob via LOCC. This task can be achieved by two steps. Firstly, create entanglement between Alice and Bob via entanglement swapping. Secondly, apply the normal teleportation protocol. Thus, it is interesting to ask the question whether there is a more efficient protocol to achieve the task.

APPENDIX: LIST OF PUBLICATIONS

The thesis is related to the following joint works with co-authors.

1. Zhaofeng Su. Generating tripartite nonlocality from bipartite resources. *Quantum Information Processing*, 16: 28, January 2017. DOI:10.1007/s11128-016-1493-7

2. Zhaofeng Su, Ji Guan, and Lvzhou Li, Efficient quantum repeater in perspective of both entanglement concentration rate and LOCC complexity, *Physical Review A*, 97:012325, January 2018. DOI: 10.1103/PhysRevA.97.012325

3. Zhaofeng Su, Lvzhou Li, and Jie Ling. An approach for quantitatively analyzing the genuine tripartite nonlocality of general three-qubit states. *Quantum Information Processing*, 17: 85, April 2018. DOI:10.1007/s11128-018-1852-7

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