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Quantum Entanglement Measures

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Abstract

An essential aspect of quantum information theory is entanglement, a property of a composite quantum system that exhibits non-local correlations between its subsystems. This property opens the door for many applications such as quantum cryptography, teleportation etc. To perform quantum computations, it is important for us to not just know if there is entanglement, but also to quantify its extent, indicating what amount of quantum information is found in the correlations rather than the constituents alone. So, the need arises for tools that quantify the entanglement, called entanglement measures. In this thesis, we first explore the nature of entanglement, how it is related to information, and we determine certain prerequisites that a good entanglement measure must satisfy. Next we begin our search of measures for bipartite systems. In the case of pure states, entanglement can be quantified by the von Neumann entropy of a subsystem's reduced density matrix, called the entropy of entanglement. If the two subsystems are qubits, we find out that the quantification of entanglement reduces to computing a simple 2×2 determinant of a coefficient matrix. However this convenience does not extend to systems larger than qubits. We proceed to examine the entanglement of mixed bipartite states, presenting two distinct approaches: operational measures such as the entanglement of formation, and geometric measures like the relative entropy of entanglement. Stepping away from bipartite systems, one encounters difficulties. When more than two parties are involved, entanglement exhibits a much richer structure, since many different partitions of the entire system are now possible. We will study the simplest generalization: a system of three qubits, which proves to be anything but simple. Even for this system, a comprehensive entanglement measure has still not been found. We introduce the 3-tangle, or three-way tangle, which quantifies what we term essential three-way entanglement among the qubits, allowing us to shed light on the distribution of entanglement among the three parties. One discovers that entangled states of three qubits fall into two inequivalent classes, named GHZ and W. States within the same class can be transformed into each other with non-zero probability via local operations and classical communication (SLOCC equivalence). Lastly, we establish significant relations satisfied by the von Neumann entropy of subsystems, with a focus on the strong subadditivity inequality (SSA).

Contents

Chapter 1

Measuring Entanglement

1.1 Entanglement and Decoherence

> *"The more important fundamental laws and facts of physical science have all been discovered, and these are so firmly established that the possibility of their ever being supplanted in consequence of new discoveries is exceedingly remote."*

This is a statement made by physicist Albert A. Michelson in 1899, which reflects the prevalent sentiment among physicists at that time. Many believed that the fundamental principles of physics were already well understood, with only minor details or "holes" remaining to be filled in. It appeared that the principles of Newtonian mechanics, Maxwell's theory of electromagnetism, and Boltzmann's statistical mechanics accounted for the majority of natural phenomena. Ironically enough, shortly after Michelson's statement, the landscape of physics underwent a dramatic transformation with the emergence of two groundbreaking theories: quantum mechanics and Einstein's theory of relativity. The former of the two, which will serve as the framework for this thesis, revolutionized our understanding of the microscopic world.

Quantum mechanics is fundamentally different form classical, Newtonian mechanics. To begin with, the classical picture of reality is deterministic. As the French mathematician Pierre-Simon Laplace famously articulated, a being with supreme intellect could, with sufficient knowledge of the present, flawlessly predict the entire future trajectory of every particle in the cosmos. In this worldview randomness is not an inherent feature; events appear random only due to our lack of knowledge. However, in quantum mechanics we have to abandon the concept of determinism, and with it, common sense altogether. In this theory, particles do not have well-defined properties, such as position or momentum, before they are measured. Instead, they exist in a state of *superposition*, meaning they can simultaneously occupy multiple states or positions. In this superposition of possibilities, it is meaningless to even define a particle's properties! As a result, even the notion of a trajectory becomes meaningless. When a measurement is made on a quantum system, the act of measurement causes the system to "collapse" into one of its possible states, and the measured properties become well-defined. The outcome of a measurement is truly probabilistic. Quantum theory is very counter-intuitive and has wild philosophical implications, but at the same time it is extremely successful at describing the behavior of particles.

The concept of superposition goes way beyond what can be described with just probability distributions. To illustrate this, let us consider a spin-1/2 particle, like an electron. The results of spin measurements along any axis are described by a wavefunction of the form

$$|\psi\rangle = a\,|\uparrow\rangle + b\,|\downarrow\rangle \tag{1.1}$$

with $|\uparrow\rangle, |\downarrow\rangle$ representing the eigenstates of spin in the chosen axis of measurement, and the coefficients $a, b \in \mathbb{C}$ satisfying the constraint $|a|^2 + |b|^2 = 1$. Measurements of the particle's spin yield the outcomes "spin-up" or "spin-down" with respective probabilities $|a|^2$ and $|b|^2$. But since the coefficients are complex numbers, these probabilities do not contain all the information present in the wavefunction. There is also a phase difference between these two numbers which can actually be measured in experiments. If we imagine that the states in (1.1) correspond to measurements in the z-axis, then we can easily compute the following expected values

$$\begin{aligned} \langle S_x \rangle &= \hbar |a||b| \cos\theta \\ \langle S_y \rangle &= \hbar |a||b| \sin\theta \\ \langle S_z \rangle &= \frac{\hbar}{2}\left(|a|^2 - |b|^2\right) \end{aligned} \tag{1.2}$$

with $\theta = \arg a - \arg b$. This evident phase dependence has no classical analogue, and gives rise to the quantum behavior of particles. It is behind the interference pattern in the famous single-particle double-slit experiment. It means the information found in the superposition exceeds that of the individual components of the sum. The wavefunction is not merely a bundle of different states in different probabilities. We call this property *coherence*, and we say that all quantum states like (1.1) are coherent.

If that wasn't strange enough, there is yet another fundamental aspect of quantum mechanics that is even more enigmatic: that of *entanglement*. Suppose we want to describe a system composed of two particles A and B. We assume that the particles have never interacted before, and they are truly independent. Then the state of the composite system is just the the product of the individual states of each particle:

$$|\psi_{AB}\rangle = |\varphi_A\rangle \otimes |\chi_B\rangle \tag{1.3}$$

But obviously not all states in the joint Hilbert space have this simple product form. Generally, a state in $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$ can be expressed as

$$|\psi_{AB}\rangle = \sum_{i=1}^{d_A} \sum_{j=1}^{d_B} a_{ij} \, |e_i^{(A)}\rangle \otimes |f_j^{(B)}\rangle \tag{1.4}$$

Here, $\{|e_i^{(A)}\rangle\}, \{|f_j^{(B)}\rangle\}$ represent basis sets of the respective Hilbert spaces and d_A, d_B their dimensions. Dividing the set of all bipartite states into product and non-product states leads us to the following definition

Definition 1.1. *A state of a bipartite system is called* ***entangled*** *if it cannot be written as a direct product of states from the individual Hilbert spaces:* $|\psi_{AB}\rangle \neq |\varphi_A\rangle \otimes |\chi_B\rangle$

The quantum state of an entangled system cannot be independently described for each constituent particle; instead, the state of one particle is intimately linked to the state of the other. This simple mathematical definition has profound physical implications. Think about a scenario where a highly energetic photon decays into an electron-positron pair: $\gamma \to e^- e^+$. In this scenario, let us introduce two distinct observers, Alice and Bob, each in possession of one of the resulting particles. While the initial photon had no spin, both particles possess a spin of 1/2. Conservation of angular momentum dictates that these particles exist in a state with zero total spin, which is known as the singlet state. Expressed in terms of the eigenstates of the individual spin operators along the z-axis, this state is represented as

$$|\chi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_A \downarrow_B\rangle - |\downarrow_A \uparrow_B\rangle\right) \tag{1.5}$$

As a matter of fact, the singlet state maintains the above form for spin eigenstates in any axis. One can easily verify that it is an entangled state, since it cannot be factorized. From its form we conclude that spin measurements will consistently reveal a correlation: whatever spin direction gets measured for one particle, the other particle has to be opposite in the same basis. Imagine, for instance, that Alice measures the spin of her particle in the z-axis and observes "spin up." In that very moment, Alice knows, with 100% certainty, that if Bob measures the spin of his particle in the same axis, he will get the result "spin-down". The remarkable aspect here is that these correlations do not necessitate physical proximity. In fact, the two observers can be arbitrarily far apart. This gives rise to a sense that causal influence might be transferred potentially faster than light. This thought experiment is termed as the “EPR paradox”, named after its discoverers Albert Einstein, Boris Podolsky and Nathan Rosen [4]. They famously objected to this idea, suggesting that quantum mechanics was incomplete and that there must be hidden variables governing the behavior of particles to preserve locality.

John Bell’s work in the 1960s [5] provided a way to test the predictions of quantum mechanics against the possibilities allowed by local hidden variables. He derived a set of mathematical inequalities, now known as *Bell’s inequalities*, that describe the correlation between measurements made on entangled particles under the assumption of local realism. Bell showed that if local hidden variables existed and determined the outcomes of measurements, the correlations between measurements on entangled particles would satisfy certain constraints. However, quantum mechanics predicts correlations that can violate these inequalities. Experimental tests of Bell’s inequalities have consistently shown that the predictions of quantum mechanics hold true, and the correlations observed between entangled particles cannot be explained by local hidden variables alone. This implies that quantum mechanics is indeed non-local in nature! Does that mean that information can travel faster than light? We should not jump to conclusions. Remember that Bob remains oblivious to the spin of his particle until he performs a measurement. And even after the measurement, he is uncertain whether the result was predetermined or truly random. The confirmation of correlated results only occurs when Alice and Bob come together or communicate classically to compare notes. As a result no real information can be transmitted instantly using entanglement. The universe conspires to avoid faster than light communication.

It is particularly interesting what happens when our focus narrows down to a subsystem within a larger, entangled system. Building upon our previous scenario, let us consider Alice’s perspective. She might be indifferent to the correlations present the entangled state, and instead be solely interested in studying the particle within her possession, with the goal of finding a mathematical tool describing its behavior. For that purpose she performs local measurements of her particle. Because this is a thought experiment, she is granted access to infinitely many copies of the same quantum system. If she had an isolated system, this process would simply yield the wavefunction of the particle. But since the system $e^- e^+$ is entangled, we know there is no state $|\psi_A\rangle$ that can adequately describe only one of the particles. And the outcomes of Alice’s measurements confirm that. Measuring the spin along any axis, there is the same 50 % probability she finds "spin up" or "spin down", meaning the expected spin in any basis is zero

$$\langle \vec{S} \cdot \vec{n} \rangle = 0 \quad \forall \quad \vec{n} \in \mathbb{R}^3 \tag{1.6}$$

which violates (1.2). Obviously this is not compatible with phase dependence, and it has significant implications. In simple terms, Alice's particle does not behave like a quantum entity! It exhibits no coherence, hence it does not by itself exist in a superposition of states. The situation is no different than flipping a classical coin: it is a random process with 50% probability of each outcome and nothing more to it. The superposition only appears when we include its entangled partner. This apparent loss of quantum behavior is observed whenever we only consider a subsystem within a larger entangled system, and it is called *decoherence*. Our capacity to observe quantum behavior depends on being able to access the entire wavefunction. We need the full picture, because coherence is not found in the individual particles, but rather in the correlations between them. On a side note, decoherence is believed to contribute to the transition from the quantum realm to the familiar macroscopic world. This transition occurs because quantum entities, despite their seeming isolation, continuously interact with countless particles in their macroscopic environment. Consequently, the network of entanglement expands rapidly, rendering it impossible to access the full wavefunction.

1.2 The Density Matrix Formalism

We have established that Alice cannot describe her entangled particle using the traditional wavefunction approach, but the initial question remains unanswered: what tool can she use to describe the properties of the particle? Here is where we introduce the concept of the density matrix. For an arbitrary quantum state $|\psi\rangle \in \mathcal{H}$ we construct the operator

$$\rho = |\psi\rangle \langle\psi| \tag{1.7}$$

known as the *density matrix* of the system. We denote the space of all the density matrices associated with the Hilbert space $\mathcal{H}$ as $\mathcal{T}(\mathcal{H})$. This operator can represent the system's properties as effectively as the state $|\psi\rangle$ itself, because statistical quantities like probabilities and expected values can be expressed through ρ using the trace operation. For an observable A with eigenvalues a_n, the probability of obtaining a_n after a measurement is

$$p_n = \mathrm{Tr}\,(\rho P_n) \tag{1.8}$$

where P_n is the projection operator onto the eigenspace corresponding to the eigenvalue a_n. Similarly, the expectation value of the observable A can be calculated as

$$\langle A\rangle = \mathrm{Tr}\,(\rho A) \tag{1.9}$$

Coherent quantum states that are described either by their wavefunction $|\psi\rangle$ or the density matrix $\rho = |\psi\rangle \langle\psi|$ are referred to as *pure states*. What about systems like Alice's particle that have lost their coherence and their "quantumness"? To understand the description of subsystems in such cases, we can draw parallels from classical mechanics. There is a concept in classical statistical mechanics that bears some resemblance to density matrices, known as the phase space distribution function. In a bipartite system AB, we can characterize subsystem A by integrating over the degrees of freedom of subsystem B in the joint distribution function ρ_{AB}:

$$\rho_A(q_A, p_A) = \int dq_B dp_B \rho_{AB}(q_A, p_A, q_B, p_B) \tag{1.10}$$

Here q_i and p_i are the generalized coordinates and momenta of the two subsystems. We apply a similar approach in our context by considering the density matrix of the entire quantum system AB and tracing out the degrees of freedom associated with Bob's particle:

$$\rho_A = \mathrm{Tr}_B \rho \tag{1.11}$$

This partial trace operation leaves us with an operator acting solely on $\mathcal{H}_A$ referred to as the *reduced density matrix* of the subsystem A. In our example, performing the partial trace produces the matrix

$$\rho_A = \frac{1}{2} |\uparrow_A\rangle \langle\uparrow_A| + \frac{1}{2} |\downarrow_A\rangle \langle\downarrow_A| = \frac{1}{2} I_A \tag{1.12}$$

We can verify that this operator successfully describes the behavior of Alice's particle, since measurement results are exactly represented by equations (1.8) and (1.9) with ρ_A replacing ρ. Here, ρ_A stands as our only tool for characterization, as there are no equivalent expressions employing a wavefunction. It is clear that this operator is a mixture of pure states: specifically, it consists of 50% the "spin up" state and 50% the"spin down" state. States that are not pure, but rather probabilistic mixtures of pure states, are called *mixed states*. They may arise from describing parts of entangled systems, although this is not their sole origin. Incomplete knowledge about the state of a system leads to a probabilistic description with a mixed state. Every mixed state can be decomposed into a convex combination of pure states, expressed as

$$\rho = \sum_i p_i |\varphi_i\rangle \langle\varphi_i| \tag{1.13}$$

with p_i denoting the probabilities associated with each pure state $|\varphi_i\rangle$, which satisfy $\sum_i p_i = 1$. Although it appears as if ρ is in diagonal form, the states $|\varphi_i\rangle$ are not necessarily orthogonal, nor do they form a basis. Also, the decomposition (1.13) is not unique, as there are infinitely many ways to represent the same mixed state as a mixture of pure states, and the number of terms in each pure-state decomposition can differ.

Any density matrix ρ, whether it describes a pure or a mixed state, has the following defining properties

1. It is a Hermitian operator: $\rho^\dagger = \rho$.
2. It is positive semi-definite: $\langle\varphi|\rho|\varphi\rangle \geq 0$ for all $|\varphi\rangle \in \mathcal{H}$. Equivalently, we can say the eigenvalues of a density matrix are always non-negative.
3. It satisfies the normalization condition $\mathrm{Tr}\,\rho = 1$.

Any operator with these properties is a valid candidate for a density matrix. From the above we conclude that a density matrix has a spectral decomposition

$$\rho = \sum_k \lambda_k |e_k\rangle \langle e_k| \tag{1.14}$$

with its eigenstates $\{|e_k\rangle\}$ forming an orthonormal basis, and the eigenvalues λ_k behaving like probabilities: they are real numbers in the range $[0, 1]$ with $\sum_k \lambda_k = 1$.

Next we will state two mathematical theorems that lie at the heart of quantum theory, and which are essential tools in our toolkit: the Schmidt decomposition of pure states and the purification theorem.

Theorem 1.2. *(Schmidt Decomposition) Suppose we have two systems A and B with dimensions of their Hilbert spaces being* $\dim \mathcal{H}_A = d_A$ *and* $\dim \mathcal{H}_B = d_B$ *respectively. Without loss of generality, we consider* $d_B \geq d_A$*. For any pure state* $|\psi_{AB}\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ *describing the whole system, there exist orthonormal sets* $\{|e_i^{(A)}\rangle\}, \{|f_i^{(B)}\rangle\}$ *such that*

$$|\psi_{AB}\rangle = \sum_{i=1}^{d_A} \sqrt{p_i}\, |e_i^{(A)}\rangle\ |f_i^{(B)}\rangle \tag{1.15}$$

Proof: In general, any pure bipartite state can be expressed in terms of basis elements of the individual Hilbert spaces as

$$|\psi_{AB}\rangle = \sum_{i=1}^{d_A} \sum_{j=1}^{d_B} a_{ij}\, |e_i^{(A)}\rangle\ |\tilde{e}_j^{(B)}\rangle \tag{1.16}$$

The reduced density matrix of subsystem A is a Hermitian operator, and as such, its eigenstates form an orthonormal basis of $\mathcal{H}_A$. We therefore have the right to use the eigenstates of ρ_A in the previous decomposition

$$\rho_A\, |e_i^{(A)}\rangle = p_i\, |e_i^{(A)}\rangle \tag{1.17}$$

We define

$$|\varphi_i^{(B)}\rangle = \sum_{j=1}^{d_B} a_{ij}\, |\tilde{e}_j^{(B)}\rangle \implies |\psi_{AB}\rangle = \sum_{i=1}^{d_A} |e_i^{(A)}\rangle\ |\varphi_i^{(B)}\rangle \tag{1.18}$$

and we obtain

$$\begin{aligned} \rho_A &= \mathrm{Tr}_B\ |\psi_{AB}\rangle\, \langle\psi_{AB}| \\ &= \mathrm{Tr}_B \left(\sum_i |e_i^{(A)}\rangle\ |\varphi_i^{(B)}\rangle \right) \left(\sum_j \langle e_j^{(A)}|\ \langle \varphi_j^{(B)}| \right) \\ &= \sum_{i,j} |e_i^{(A)}\rangle\, \langle e_j^{(A)}|\ \langle \varphi_i^{(B)} | \varphi_j^{(B)}\rangle \end{aligned} \tag{1.19}$$

Given our choice in (1.17), this is just the spectral decomposition of ρ_A and should be equal to $\rho_A = \sum_i p_i\, |e_i^{(A)}\rangle\, \langle e_i^{(A)}|$. We conclude that the states $|\varphi_i^{(B)}\rangle$ must be orthogonal, with squared magnitude p_i

$$\langle \varphi_j^{(B)} | \varphi_i^{(B)}\rangle = \delta_{ji} p_i \tag{1.20}$$

If we denote with $|f_i^{(B)}\rangle$ the respective normalized states, we finally arrive at

$$|\psi_{AB}\rangle = \sum_{i=1}^{d_A} |e_i^{(A)}\rangle\ |\varphi_i^{(B)}\rangle = \sum_{i=1}^{d_A} \sqrt{p_i}\,|e_i^{(A)}\rangle\ |f_i^{(B)}\rangle \quad \blacksquare \tag{1.21}$$

We can make some interesting observations. As was stated in the above proof, the set $\{|e_i^{(A)}\rangle\}$ that appears in the Schmidt decomposition is the set of ρ_A's eigenvectors, with p_i being the corresponding eigenvalues. This property is not unique to subsystem A: the states in the set $\{|f_i^{(B)}\rangle\}$ are the eigenvectors of ρ_B, and interestingly enough, they share the exact same eigenvalues:

$$\begin{aligned}\rho_A &= \mathrm{Tr}_B\,\rho_{AB} = \sum_{i=1}^{d_A} p_i\,|e_i^{(A)}\rangle\,\langle e_i^{(A)}| \\ \rho_B &= \mathrm{Tr}_A\,\rho_{AB} = \sum_{i=1}^{d_A} p_i\,|f_i^{(B)}\rangle\,\langle f_i^{(B)}|\end{aligned} \tag{1.22}$$

There is, however, one major difference: the sum in the expression for ρ_B only goes up to $d_A \leq d_B$. Hence, ρ_B does not utilize the full Hilbert space, as it has at most d_A non-zero eigenvalues. Only the d_A-dimensional eigenspace of the density matrix is necessary to express an arbitrary state of AB. This is a consequence of coupling two systems of different sizes: put simply, the large system behaves like a system with the size of its smaller partner.

While the Schmidt decomposition is always at one's disposal when it comes to bipartite systems, there is no analogous statement for larger systems. Even for systems with just three parties, A,B and C, there is no general prescription, according to which, we can write

$$|\psi_{ABC}\rangle = \sum_i \sqrt{p_i}\,|e_i^{(A)}\rangle\ |f_i^{(B)}\rangle\ |g_i^{(C)}\rangle \tag{1.23}$$

with $\{|e_i^{(A)}\rangle\}, \{|f_i^{(B)}\rangle\}$ and $\{|g_i^{(C)}\rangle\}$ being orthonormal sets. But still, nothing is stopping us from considering that A and B constitute a single system, and then the Schmidt decomposition holds for the bipartite system AB-C

$$|\psi_{ABC}\rangle = \sum_i \sqrt{p_i}\,|e_i^{(AB)}\rangle\ |f_i^{(C)}\rangle \tag{1.24}$$

and consequently, the respective density matrices ρ_{AB} and ρ_C have equal eigenvalues.

Theorem 1.3. *(Purification) Suppose we are given a (generally mixed) state ρ_A describing a system A. It is always possible to consider this state as a result of a partial trace operation on a larger system AS in a pure state $|\psi_{AS}\rangle$. The actual physical origin of ρ_A might be completely different, but we can always conceptualize it as arising from looking at a subsystem of a larger system in a pure, generally entangled state.*

Proof This procedure is purely mathematical, and is closely related to the Schmidt decomposition. An arbitrary mixed state has a spectral decomposition

$$\rho_A = \sum_{i=1}^{d_A} p_i\,|e_i\rangle\,\langle e_i| \tag{1.25}$$

with $\{|e_i\rangle\}$ being orthonormal. To prove that purification is possible, we introduce an auxiliary system S, and an orthonormal set $\{f_i^{(S)}\}$ of $\mathcal{H}_S$. For the purpose of this discussion, we assume that $\dim \mathcal{H}_S \geq d_A$. We define a pure state $|\psi_{AS}\rangle$ of the composite system AS by assigning an element of this set to each state of the sum (1.25), essentially constructing the Schmidt decomposition of $|\psi_{AS}\rangle$

$$|\psi_{AS}\rangle = \sum_{i=1}^{d_A} p_i \, |e_i^{(A)}\rangle \, |f_i^{(S)}\rangle \tag{1.26}$$

Then it is simple to see

$$\rho_A = \mathrm{Tr}_S \, |\psi_{AS}\rangle \, \langle\psi_{AS}| = \sum_{i=1}^{d_A} p_i \, |e_i\rangle \, \langle e_i| \quad \blacksquare \tag{1.27}$$

1.3 Entanglement Can Be Quantified

Studying the spectral decomposition of a system's density matrix can reveal valuable information about the system. The rank of a density matrix, i.e. the number of its non-zero eigenvalues, is known as the *Schmidt number* K of the matrix. It represents the minimum number of terms in any one of its pure-state decompositions. Pure states have only one non-zero eigenvalue, which is equal to 1. Mixed states correspond to numbers $1 < K \leq d$, where d represents the dimension of the Hilbert space. Thus, the Schmidt number serves as a distinguishing factor between pure and mixed states. However, determining the Schmidt number for a given state can be challenging. Thankfully, we have a simpler tool at our disposal. We define the *purity* $\mathcal{P}$ of a density matrix ρ to be the quantity

$$\mathcal{P} = \mathrm{Tr}\,\rho^2 \tag{1.28}$$

For pure states, the square of the density matrix is identical to the original matrix itself: $\rho^2 = \rho$. From the normalization condition it then follows that such states have purity of 1. But that is not the case in general. For mixed states we can compute that

$$\mathcal{P} = \sum_k \lambda_k^2 < 1 \tag{1.29}$$

We can also find that purity has a lower bound of $1/d$, and putting all the above together we obtain

$$\frac{1}{d} \leq \mathcal{P} \leq 1 \tag{1.30}$$

with $\mathcal{P} = 1$ if and only if the state is pure. Purity values of less than 1 indicate mixing between states. This observation serves as a criterion for distinguishing between pure and mixed states. But there is also an underlying element of quantification. As purity decreases from 1, the degree of mixing increases, signifying greater uncertainty about the state of the system. A state like (1.12), that is proportional to the identity matrix, and with minimum purity $\mathcal{P} = 1/d$, is a maximally mixed state. It is a perfect mixture, because all possible states are equally probable

with a probability of $1/d$.

The preceding discussion invites us to explore further. Imagine a bipartite system in a pure, entangled state $|\psi\rangle$. We know that the act of describing only a part of the composite system creates decoherence, resulting in a mixed state. However, as we discussed, it makes sense to talk about the extent of mixing within a mixed state. This prompts the question: since the mixture is the result of entanglement, can the degree of mixing be interpreted as the degree of entanglement present in the initial state $|\psi\rangle$? Is entanglement itself something that can be quantified? The answer is yes. The rest of this thesis is dedicated to the search of *entanglement measures*, functions that are able to quantify the entanglement in a given quantum state. But before we mention anything else, we need to talk about a small elephant hanging around in the room. Up to this point we have only addressed the entanglement of pure states. But can't mixed states also exhibit quantum correlations? They absolutely can, meaning we need to expand the definition of entanglement to include mixed states.

Pure states are either uncorrelated (factorized) or entangled. Any correlations have strictly quantum origin, and cannot be produced locally by two separate observers. Mixed states, however, introduce a more nuanced perspective. Of course, it's easy to conceive of a mixed state with no correlations at all: any product state $\rho = \rho_A \otimes \rho_B$ where Alice and Bob own each a separate state qualifies as such. But are we justified in labeling any non-product state as entangled? Lets consider the next scenario. Imagine Alice and Bob share a random number generator via classical communication, yielding outcomes i with probabilities p_i. For each outcome, they agree to produce the state $\rho_i^A \otimes \rho_i^B$ locally. Through this process, they generate the state:

$$\rho = \sum_i p_i \rho_i^A \otimes \rho_i^B \tag{1.31}$$

It is clear that there are correlations present in this state, but there is nothing inherently quantum in the above procedure. These are classical correlations, generated through local operations assisted by classical means of communication (LOCC). Mixed states that can be expressed as a convex combination of product states, as shown in the above equation, are termed *separable*. Any correlations beyond this framework are indeed quantum in nature. Thus, if a state is not separable, we classify it as *entangled*.

Definition 1.4. *A mixed state is* ***entangled*** *if it cannot be expressed as a convex sum of product states as in* (1.31).

Now that we've gained a comprehensive understanding of entanglement for all states, we can focus on our objective of finding entanglement measures. We define an entanglement measure $E(\rho)$ to be a mapping $E : \mathcal{H} \to \mathbb{R}^+$ with a physical or mathematical justification for claiming that it quantifies the amount of entanglement in a state. Furthermore, it has to be consistent with the behavior of entanglement under different classes of quantum operations. This requirement gives rise to conditions that are necessary and universal for all entanglement measures. Before we examine these conditions, we first need a clear framework of the classes of quantum operations themselves.

1.4 Quantum Operations

Quantum operations $\mathcal{E}(\rho)$ (also known as quantum channels) are maps that describe the dynamics of quantum systems. We restrict ourselves to linear, completely positive and trace-preserving

(CPTP) maps from the set of density matrices into itself. A unitary evolution is a special case of such operations

$$\mathcal{E}(\rho) = U\rho U^\dagger \tag{1.32}$$

with U being a unitary operator. But generally quantum operations can also describe non-unitary evolutions, which can be represented by operator sums as

$$\mathcal{E}(\rho) = \sum_k M_k \rho M_k^\dagger \tag{1.33}$$

The set of operators $\{M_k\}$ satisfy the completeness relation $\sum_k M_k^\dagger M_k = I$, and are called *Krauss operators*. One interpretation of non-unitary evolutions is the following: we suppose our system in the initial state $\rho(0)$ is coupled with an environment in a pure state $|\psi_0\rangle$. If we allow for interactions between our system and the environment, then the entire system has a unitary evolution in time $U(t)$. To obtain the state of the system after some time t, we first perform the unitary evolution on the entire system, and then trace out all the environmental degrees of freedom by summing over an orthonormal set $\{|e_k\rangle\}$ of the environment

$$\rho(t) = \mathrm{Tr}_{env}\left\{U(t)\,|\psi_0\rangle\,\langle\psi_0|\,\rho(0)U^\dagger(t)\right\} \tag{1.34}$$

The result is exactly an operator sum representation

$$\rho(t) = \sum_k M_k \rho_0 M_k^\dagger \tag{1.35}$$

with $M_k = \langle e_k|U(t)|\psi_0\rangle$.

Now lets focus on composite systems, and specifically on bipartite systems for simplicity. A particular class of operations acting on such systems are *local operations*. These are performed by the two parties separately, and thus are described by two sets of Krauss operators. The joint action of these on a state ρ is of the form

$$\Lambda(\rho) = \sum_{i,j} A_i \otimes B_j \rho A_i^\dagger \otimes B_j^\dagger \tag{1.36}$$

with $\sum_i A_i^\dagger A_i = I_A$ and $\sum_i B_j^\dagger B_j = I_B$. Because the two subsystems evolve independently from each other, any correlations present in the state ρ cannot be affected. Product states remain as such, and any separable state retains its separability under local operations. Therefore local operations cannot be used to create entanglement.

Any quantum operation that is not local is referred to as *global*. One particular subset of global operations that we have already mentioned is *local operations and classical communication (LOCC)*. These operations involve local transformations as described earlier, along with allowing the involved parties to communicate with each other through classical means. This setup enables the establishment of correlations, as both parties can exchange information and coordinate their actions. For instance, when Alice applies operator A_i in her subsystem, Bob can respond with B_i. The collective action on the entire system is depicted as:

$$\Lambda(\rho) = \sum_i A_i \otimes B_i \rho A_i^\dagger \otimes B_i^\dagger \tag{1.37}$$

The correlated application of the operations is evident, as there only a single sum involved. LOCC operations are completely positive maps, and to ensure that they are also trace preserving, we require $\sum_i A_i^\dagger A_i \otimes B_i^\dagger B_i = I$. Even though correlations can be produced, they are exclusively classical in nature. For that reason, LOCC operations cannot be used to create entanglement.

1.5 Conditions for Entanglement Measures

We can conceive of certain prerequisites that must be satisfied for a quantity to be considered a viable entanglement measure. From what we have discussed up until this point, we conclude that the following conditions are absolutely necessary for any entanglement measure $E(\rho)$:

1. $E(\rho) = 0$ if and only if the state ρ is separable.
2. The measure is invariant under local unitary (LU) transformations $U = U_A \otimes U_B$:

$$E(\rho) = E(U_A \otimes U_B \rho U_A^\dagger \otimes U_B^\dagger) \tag{1.38}$$

3. The measure cannot increase under any LOCC Λ:

$$E(\rho) \geq E(\Lambda\rho) \tag{1.39}$$

There is solid justification for each condition. The first one is self-evident for the consideration of $E(\rho)$ as an entanglement measure. Sometimes in the literature we meet the formulation "$E(\rho) = 0$ *if* ϱ *is separable*", but we adhere to the stronger version. The second condition stems from the fact that LU transformations merely represent local changes in basis, and should thus leave any quantum correlations intact. The origin of the third condition is that LOCC operations can be used to increase only classical correlations, and as a result entanglement should not be increased this way. This condition is known as *monotonicity*, and quantities that satisfy it are called *entanglement monotones*. Usually entanglement measures satisfy a stronger version of monotonicity: when the result of a LOCC operation is an ensemble of states $\{p_k, \rho_k\}$ the entanglement measure does not increase on average [6]

$$E(\rho) \geq \sum_k p_k E(\rho_k) \tag{1.40}$$

This condition was at one point considered mandatory, but now there is common agreement that only (1.39) is necessary. Interestingly enough, it is often easier to prove this stronger version of monotonicity.

It was proven by Vidal [7] that the restriction of entanglement monotones on pure states $|\psi\rangle$ is given by a function of the partial trace $\rho_A = \mathrm{Tr}_B |\psi\rangle \langle\psi|$

$$E(\psi) = h(\rho_A) \tag{1.41}$$

that is i) unitarily invariant and ii) a concave function, meaning that

$$h\left[\lambda\rho_1 + (1-\lambda)\rho_2\right] \geq \lambda h(\rho_1) + (1-\lambda)h(\rho_2) \tag{1.42}$$

for all $\lambda \in [0,1]$ and density matrices $\rho_1, \rho_2 \in \mathcal{T}(\mathcal{H}_A)$. Hence, whenever we study entanglement measures for pure states, these are the requirements that must be met. Again, we can consider a stronger monotonicity condition: it is often enough to require that local measurements do not increase the average entanglement when we transition from a pure state to an ensemble of pure states $|\psi\rangle \to \{p_i, |\psi_i\rangle\}$

$$E(\psi) \geq \sum_i p_i E(\psi_i) \tag{1.43}$$

where $|\psi_i\rangle$ are obtained from the local operation

$$|\psi_i\rangle = \frac{V_i|\psi\rangle}{||V_i\psi||} \tag{1.44}$$

and $V_i = A_i \otimes I$ (or $V_i = I \otimes B_i$) are Krauss operators of a local measurement satisfying $\sum_i V_i^\dagger V_i = I$, and p_i are probabilities of outcomes.

It is important to point out that monotonicity of an entanglement measure actually implies its LU invariance. Local unitary operations $U = U_A \otimes U_B$ constitute a subset of LOCC operations, hence monotonicity applies. For the operation $\rho \to \rho' = U\rho U^\dagger$ we obtain

$$E(\rho) \geq E(\rho') \tag{1.45}$$

Such transformations are invertible, and the inverse of a unitary operator is simply its Hermitian conjugate: $U^{-1} = U^\dagger = U_A^\dagger \otimes U_B^\dagger$. Therefore, if Alice and Bob regret their decision to apply a particular LU operation, they can simply reverse their action locally: $\rho' \to U^\dagger \rho' U = \rho$. Again, this constitutes another LOCC operation, so

$$E(\rho') \geq E(\rho) \tag{1.46}$$

The only way to reconcile (1.45) with (1.46) is if equality strictly holds. As a result, monotonicity directly implies LU invariance. Although redundant, both conditions are usually mentioned as necessary for entanglement measures in the literature. A reason could be that LU invariance is easier to check than monotonicity, and if that check fails, it can immediately disqualify a potential candidate for an entanglement measure.

Of course we can keep the discussion going; there are many thing that can be said about the expected behavior of entanglement measures. For example, good entanglement measures are *convex*, meaning that for any two states $\rho_1, \rho_2 \in \mathcal{T}(\mathcal{H})$, and for all $\lambda \in [0,1]$

$$E\left[\lambda\rho_1 + (1-\lambda)\rho_2\right] \leq \lambda E(\rho_1) + (1-\lambda)E(\rho_2) \tag{1.47}$$

The underlying physics behind this principle is the following: imagine that we have two pairs of particles in the mixed state ensemble $\{\lambda, \rho_1; 1-\lambda, \rho_2\}$. If information about the system is lost, rendering the association of states with physical pairs impossible, each pair effectively transitions into the mixed state $\rho = \lambda\rho_1 + (1-\lambda)\rho_2$. This process of discarding information is called *mixing*, and can be done locally. Hence, (1.47) can be interpreted as the monotonicity condition of an entanglement measure for the transformation $\{\lambda, \rho_1; 1-\lambda, \rho_2\} \to \rho = \lambda\rho_1 + (1-\lambda)\rho_2$. When we mix quantum states we should not end up with more entanglement than what we originally had.

Chapter 2

Pure States of Bipartite Systems

2.1 Entropy of Entanglement

Let us attempt to view entanglement and decoherence fro a different perspective. This can be achieved with the help of a concept from information theory known as *Shannon entropy*. Consider a discrete random variable X, with outcomes X_i and respective probabilities p_i. The Shannon entropy of this variable is defined as

$$H(X) = -\sum_i p_i \log_2 p_i \tag{2.1}$$

This quantity can be interpreted as measuring the uncertainty or the disorder of a probability distribution. Maximum uncertainty is achieved for uniform distributions, where all the outcomes have equal probability. This is the case of complete randomness and disorder. Distributions where we have some degree of certainty about the outcome, like for example with loaded dice, correspond to less entropy. And in the extreme case where there is only one non-zero probability, then the outcome of an event is certain and its entropy is zero.

Now let us bring Shannon entropy into the context of entanglement. A mixed state $\rho = \sum_i p_i |\varphi_i\rangle \langle\varphi_i|$ can be seen as representing a quantum random variable whose outcomes are the pure quantum states $|\varphi_i\rangle$. Defining the entropy of this quantum variable is not trivial. We have to be careful, because now the outcomes are not necessarily discrete, i.e. the states $|\varphi_i\rangle$ are not always orthogonal. However, any mixed state can be decomposed into orthogonal pure states using its spectral decomposition: $\rho = \sum_i \lambda_i |e_i\rangle \langle e_i|$. For this particular distribution the Shannon entropy can be defined, and it has a special name.

Definition 2.1. *We define the* ***von Neumann entropy***[1] *of a density matrix ρ to be quantity*

$$S(\rho) = -\operatorname{Tr} \rho \log_2 \rho = -\sum_i \lambda_i \log_2 \lambda_i \tag{2.2}$$

We have adopted the convention of using the base-2 logarithm, however the natural logarithm can be used just as well to define the entropy. For simplicity, we will omit specifying the base in the logarithm going forward, while maintaining our preference for the base-2 logarithm. This entropy measures the disorder of the eigenvalues of the density matrix. Another useful perspective on entropy is through the lens of information theory. Shannon entropy can be thought of as the amount of hidden information in a system, or more precisely, the amount of information we can hope to gain by making a measurement of the system. In a random

[1] named after the Hungarian mathematician and physicist John von Neumann

experiment, greater uncertainty about the outcome implies more hidden information, which can be unveiled by a measurement. As far as two-outcome events are concerned, flipping a coin corresponds to maximum Shannon entropy $H(\text{coin}) = 1$, because both outcomes are equally likely. We essentially know nothing about the coin's state until we perform a measurement. If somehow the coin had a preference, say for example "heads" had a probability of $p > 1/2$ then this would be a lower entropy event, with

$$H(p) = -p \log p - (1 - p) \log (1 - p) \tag{2.3}$$

The above expression is known as the *binary entropy function*. But what happens if we have a "quantum coin"? Imagine a spin 1/2 particle in the state $|\psi\rangle = (|\uparrow\rangle + |\downarrow\rangle) / \sqrt{2}$, which has an equal 50% probability of yielding "spin up" or "spin down" upon measurement. This is fundamentally different from what we previously described. The result of flipping a regular coin is entirely *heads or tails*, and appears as a random event to us due to our lack of information about its current state. But in quantum mechanics, the wavefunction contains all the information there is to know about a system. When the quantum coin is flipped, it is in a superposition of *heads and tails*. Here, we possess complete knowledge of the system's state, and no hidden information exists. Observing the coin doesn't uncover new information but rather causes a (truly) random change in its state. Consequently, the entropy of any pure quantum state is zero. This conclusion is confirmed by the formula for the von Neumann entropy, as pure states have only one non-zero eigenvalue $\lambda = 1$.

Now lets bring entanglement into the picture and consider the familiar example of the singlet state $|\psi\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) / \sqrt{2}$. This is a pure state, and as such it has zero von Neumann entropy. Any observer with access to both particles has full knowledge of the system, and observes quantum behavior like superposition. But we know what happens when we only have access to one of the particles: decoherence. When viewed in isolation, any of the particles behaves classically, and is indistinguishable from a classical coin. It is in a mixed state of *either "spin up" or "spin down"*, each with 50% probability. Information is now hidden. It is hidden in the correlations that are found in the entangled wavefunction. We therefore went from a pure state with all the information available, to an incomplete description, where information is hidden. We conclude that the consequence of decoherence is *loss of quantum information*. This lost information is precisely quantified by the von Neumann entropy of the reduced density matrix describing one of the two subsystems. It is then safe to say that the von Neumann entropy quantifies the quantum correlations in the singlet state. But this is just another way of saying that it quantifies *the entanglement* of the state. Based on this argument, we feel confident enough to present the first candidate for a measure of entanglement for pure, bipartite states:

Definition 2.2. *For any pure bipartite quantum state $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ we define the* ***entropy of entanglement*** *as the von Neumann entropy of the reduced density matrix describing a subsystem*

$$E(\psi) = S(\rho_A) = -\operatorname{Tr} \rho_A \log \rho_A \tag{2.4}$$

Here, $\rho_A = \operatorname{Tr}_B |\psi\rangle \langle\psi|$. It is important to note that the choice of the subsystem to be traced out is arbitrary. This is because the von Neumann entropy depends solely on the eigenvalues of a density matrix, and it has been previously demonstrated that ρ_A and ρ_B share identical eigenvalues, resulting in $S(\rho_A) = S(\rho_B)$.

When evaluating a candidate for an entanglement measure we must first check whether it meets the prerequisites outlined in section 1. It is clear that $S(\rho_A) = 0$ if and only if ρ_A is a pure state, or equivalently, if $|\psi\rangle$ is a product state. Now, is the entropy of entanglement a monotone? Since we are proposing a measure for pure states, this task boils down to confirming that the von Neumann entropy i) remains invariant under unitary transformations and ii) is a concave function. The first of these two conditions follows immediately from the invariance of the trace of a matrix under unitary transformations. For $\rho = \lambda\rho_1 + (1-\lambda)\rho_2$ we obtain

$$\begin{aligned} S(\rho) &= -\operatorname{Tr}\{[\lambda\rho_1 + (1-\lambda)\rho_2]\log[\lambda\rho_1 + (1-\lambda)\rho_2]\} \\ \implies \frac{\partial S}{\partial \lambda} &= -\operatorname{Tr}\{(\rho_1 - \rho_2)\log[\lambda\rho_1 + (1-\lambda)\rho_2] + \rho_1 - \rho_2\} \\ \implies \frac{\partial^2 S}{\partial \lambda^2} &= -\operatorname{Tr}\left\{\frac{(\rho_1 - \rho_2)^2}{\lambda\rho_1 + (1-\lambda)\rho_2}\right\} \leq 0 \end{aligned} \tag{2.5}$$

The inequality for the second derivative holds because density matrices are positive semi-definite operators, meaning this trace is non-negative. We thus conclude that $S(\rho)$ is indeed a concave function. ■

We have made significant progress. First we introduced the entropy of entanglement from an information-theoretic standpoint and established its direct connection with decoherence, and by extension, with entanglement. Furthermore, we verified that it behaves in accordance with the characteristics expected of an entanglement measure. This measure categorizes all pure bipartite states along a spectrum. At one end, we encounter uncorrelated product states, while at the other end, we find states like the singlet, which exhibit maximal entanglement. Notably, the singlet state is part of a renowned set of four maximally entangled states known as the *Bell states*. These states describe particles that are entirely correlated, and they are the following

$$\begin{aligned} |\varphi^+\rangle &= \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \\ |\varphi^-\rangle &= \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle) \\ |\psi^+\rangle &= \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) \\ |\psi^-\rangle &= \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle) \end{aligned} \tag{2.6}$$

For anyone that is not convinced yet about the asserted role of the entropy of entanglement, the next section will dispel any remaining doubts, by proving that it qualifies as what we term an *operational measure*.

2.2 Entanglement Distillation and Dilution

Quantum protocols often rely on two parties sharing highly entangled states like the Bell states. But what if they simply do not have Bell states at their disposal? The Schmidt decomposition guarantees that we can write an arbitrary pure state of two qubits as

$$|x_{AB}\rangle = \sqrt{p}\,|00\rangle + \sqrt{1-p}\,|11\rangle \tag{2.7}$$

which is generally entangled, but not to the fullest extent. We know that there is nothing observers can do locally to transform this state into a maximally entangled one, since entanglement does not increase through local manipulations. Instead let us suppose Alice and Bob share n copies of the above state. We want to answer the following question: how many maximally entangled states can be produced by applying LOCC to these n states that are not fully entangled? The motivation behind this question is on one hand practical, because we want to work with Bell-like states. But on the other hand, the answer equips us with a tool to quantify entanglement: if we are able to extract $m < n$ maximally entangled states, then the ratio m/n informs us of the "weight" of entanglement carried by the state $|x_{AB}\rangle$. An oversimplified analogy could be the gold purity of a metal alloy, with 24K gold corresponding to maximally entangled states. This process, which is known as *entanglement distillation*, comes with a cost: we have to pay the price of $n-m$ copies of the initial state, and obviously, less entangled states will require a higher price.

This joint system of the n pairs of particles is described by the product state vector

$$|x_{AB}\rangle^{\otimes n} = \sum_{k=0}^{n} (\sqrt{p})^k \left(\sqrt{1-p}\right)^{n-k} |\tilde{x}_{AB}^{(k)}\rangle \tag{2.8}$$

with the subscript next to each ket denoting the pair of particles it refers to, and $|\tilde{x}_{AB}\rangle^{(k)}$ encompasses all the states with zeros appearing k times and ones $n-k$ times

$$|\tilde{x}_{AB}^{(k)}\rangle = |00\rangle_1 \, |00\rangle_2 \cdots |00\rangle_k \, |11\rangle_{k+1} \cdots |11\rangle_n + \text{permutations} \tag{2.9}$$

The permutations include all the possible ways to choose k zeros from a total of n pairs, thus we get $\binom{n}{k}$ terms that are orthonormal. By denoting $|x_{AB}^{(k)}\rangle$ the respective normalized state, we write

$$|x_{AB}\rangle^{\otimes n} = \sum_{k=0}^{n} \sqrt{\binom{n}{k}} (\sqrt{p})^k \left(\sqrt{1-p}\right)^{n-k} |x_{AB}^{(k)}\rangle = \sum_{k=0}^{n} C_k \, |x_{AB}^{(k)}\rangle \tag{2.10}$$

Having prepared this state, we now suppose that Alice performs measurements on her share of particles. Specifically we consider the case where she measures the component of the spin in the z-axis, of all the particles that belong in her system. Mathematically this quantity is described by the operator $M_{AB} = \sigma_{z,A}^{total} \otimes I_B$, with $\sigma_{z,A}^{total} = \left(\sigma_z^A\right)_1 + \left(\sigma_z^A\right)_2 + \cdots + \left(\sigma_z^A\right)_n$. Quite conveniently, each state $|x_{AB}^{(k)}\rangle$ is an eigenstate of this operator, with the corresponding eigenvalue being[2] $\sigma_{z,A}^{total} = k\,(+1) + (n-k)\,(-1) = 2k - n$. The probability that a measurement yields this value is $|C_k|^2$ for each k. We will now study the behavior of these probabilities for a large number of copies n, but also large values of k. We start by writing $C_k = A_k B_k$ with

$$A_k = (\sqrt{p})^k \left(\sqrt{1-p}\right)^{n-k} \quad \text{and} \quad B_k = \sqrt{\binom{n}{k}} \tag{2.11}$$

It is

$$\log A_k = \frac{n}{2}\left[\frac{k}{n}\log p + \frac{n-k}{k}\log(1-p)\right] \tag{2.12}$$

[2] we assign the value +1 to $|0\rangle$ and -1 to $|1\rangle$.

The law of large numbers dictates that the ratio k/n approaches the probability of yielding the result 0 in a measurement of an individual state, which none other than p. Similarly the ratio $(n-k)/n$ approaches the probability of yielding 1, which is equal to $1-p$. Consequently

$$A_k = \left(\sqrt{p}\right)^k \left(\sqrt{1-p}\right)^{n-k} \approx 2^{-\frac{n}{2}H(p)} \tag{2.13}$$

where $H(p) = -p\log p - (1-p)\log(1-p)$. The other part of the coefficients C_k is

$$B_k = \sqrt{\binom{n}{k}} = \sqrt{\frac{n!}{(n-k)!\,k!}} \tag{2.14}$$

By taking the logarithm and using Stirling's approximation for large numbers, we obtain

$$\begin{aligned}
\log B_k &= \frac{1}{2}\left[\log n! - \log(n-k)! - \log k!\right] \\
&\approx \frac{1}{2}\left[n\log n - (n-k)\log(n-k) - k\log k\right] \\
&= -\frac{n}{2}\left[\frac{k}{n}\log\frac{k}{n} + \frac{n-k}{n}\log\frac{n-k}{n}\right]
\end{aligned} \tag{2.15}$$

The argument from the law of large numbers can also be applied here, giving $B_k \approx 2^{\frac{n}{2}H(p)}$. This is a very important result. We demonstrated that for a large number n, there is a particular (large) value of k, for which

$$C_k \approx 2^{\frac{n}{2}H(p)}\, 2^{-\frac{n}{2}H(p)} = 1 \tag{2.16}$$

The implication of this statement is that, in the sum (2.10), there is one term that appears with probability very close to 1. As a matter of fact, this probability can be arbitrarily close to 1, if n is chosen to be sufficiently large. This highly probable term corresponds to the value $k = np$. Therefore, right after Alice measures the quantity M_{AB}, the initial product state collapses, almost certainly, to the state

$$|x_{AB}^{(k)}\rangle = \frac{1}{\sqrt{\binom{n}{k}}}\left\{\prod_{i=1}^{k}|00\rangle_i \prod_{j=k+1}^{n}|11\rangle_j + \text{permutations}\right\} \tag{2.17}$$

where k takes the particular value np. Using Shannon's terminology, we essentially get a *typical sequence*. We showed that the normalization factor is approximately $2^{-\frac{n}{2}H(p)}$, with $H(p) = -p\log p - (1-p)\log(1-p)$. We see that the expression for the binary entropy has emerged, but what is the interpretation? To answer, we have to return to the bipartite state that was used in the beginning of this protocol. The state $|x_{AB}\rangle$ in (2.7) is written in the Schmidt decomposition, meaning that p and $1-p$ are the eigenvalues of the reduced density matrices of the respective subsystems. Hence, the function $H(p)$ represents the von Neumann entropy of the subsystems

$$H(p) = -p\log p - (1-p)\log(1-p) = S(\rho_A) \tag{2.18}$$

For each pair we make the substitutions

$$\begin{aligned} |00\rangle_i &= \frac{1}{\sqrt{2}}\left(|\varphi^+\rangle_i + |\varphi^-\rangle_i\right) \\ |11\rangle_i &= \frac{1}{\sqrt{2}}\left(|\varphi^+\rangle_i - |\varphi^-\rangle_i\right) \end{aligned} \tag{2.19}$$

$$\begin{aligned} |x_{AB}^{(k)}\rangle &= \frac{1}{2^{\frac{nS}{2}}}\left\{\prod_{i=1}^{k}|00\rangle_i \prod_{j=k+1}^{n}|11\rangle_j + \text{permutations}\right\} \\ &= \frac{1}{2^{\frac{nS}{2}}2^{\frac{n}{2}}}\left\{\prod_{i=1}^{k}\left(|\varphi^+\rangle_i + |\varphi^-\rangle_i\right)\prod_{j=k+1}^{n}\left(|\varphi^+\rangle_j - |\varphi^-\rangle_j\right) + \text{permutations}\right\} \\ &= \frac{1}{2^{\frac{nS}{2}}2^{\frac{n}{2}}}\left\{\binom{n}{k}\prod_{i=1}^{n}|\varphi^+\rangle_i + (-1)^{n-k}\binom{n}{k}\prod_{i=1}^{n}|\varphi^-\rangle_i + \text{cross terms}\right\} \\ &= \frac{1}{2^{-\frac{nS}{2}}2^{\frac{n}{2}}}\prod_{i=1}^{n}|\varphi^+\rangle_i + \frac{(-1)^{n-k}}{2^{-\frac{nS}{2}}2^{\frac{n}{2}}}\prod_{i=1}^{n}|\varphi^-\rangle_i + \ldots \end{aligned} \tag{2.20}$$

The cross terms include all the combinations where both Bell states appear in different numbers. Because of cancellations, the number of identical cross terms is always less than $\binom{n}{k} \approx 2^{nS}$. The next step in our protocol involves Alice sending one of her particles over to Bob, for example the particle from pair number 1. Now, Bob being the owner of a whole pair, can perform joint measurements on these two particles. After a Bell measurement, the state of the first pair is projected to either $|\varphi^+\rangle_1$ or $|\varphi^-\rangle_1$. For the sake of argument, suppose he finds the state $|\varphi^+\rangle_1$. Then, from all the terms in (2.20) only half survive, namely, those that begin with $|\varphi^+\rangle_1$. We disregard the first pair[3] and focus on the remaining $n-1$ that Alice and Bob still share. The state that describes this system, in order to be normalized, has to be multiplied by a factor of $\sqrt{2}$, since it contains half the terms compared to $|x_{AB}\rangle$.

This process gets repeated many times: Alice keeps sending particles and after each measurement by Bob the coefficients of the remaining states are multiplied by $\sqrt{2}$. After a number of transmitted particles we will eventually reach the end goal, which is to attain a single product state composed of maximally entangled Bell states. Let us denote that number as x. The total factor of $2^{\frac{x}{2}}$ makes the coefficient of that final state equal to 1. Obviously, different states in the sum (2.20) have generally different coefficients, thus the number of required particles differs depending on the final state. We are interested in the optimal rate at which Alice and Bob can convert partially entangled states to Bell states. The state that can be reached with the minimum number of particles is the one with the largest coefficient, for which

$$\frac{2^{\frac{x}{2}}}{2^{-\frac{nS}{2}}2^{\frac{n}{2}}} = 1 \implies x = n - nS \tag{2.21}$$

[3] we can because it is factored out

This constitutes the minimum price that has to be payed to convert the initial n copies of the state $|x_{AB}\rangle$ into maximally entangled states. After a successful implementation of the protocol we have extracted $m = n - x = nS$ Bell states. The ratio m/n is equal to

$$\frac{m}{n} = S(\rho_A) \tag{2.22}$$

and is referred to as *distillable entanglement* E_D. It expresses the amount of entanglement carried by a single bipartite state $|x_{AB}\rangle$, and we proved that it is equal to the von Neumann entropy of one subsystem, or equivalently, the entropy of entanglement of $|x_{AB}\rangle$. although we specifically discussed a protocol for two-qubit systems, the underlying principle applies to bipartite states of any dimension.

One might wonder if the reverse process is possible, and if so, whether it has any physical significance. Let us imagine that we start again with two separated observers, but this time they share a large number m of maximally entangled Bell states. Is it possible to convert these into n copies of a particular state $|x_{AB}\rangle$ through LOCC? The answer is yes, and the process through which we achieve this is called *entanglement dilution*. There is, same as before, a price to be paid: our two observers must use up a minimum number of the initial Bell states in order to successfully produce the desired copies of $|x_{AB}\rangle$. It can be shown that this number approaches $nE(x_{AB})$ asymptotically close, for sufficiently large m, n. If we define the entanglement of a Bell state to be equal to one "ebit", then the number of ebits required to prepare a single copy of a pure of the state using only LOCC operations, known as the *entanglement cost* E_C, is precisely the entropy of entanglement $E(x_{AB})$. Thus, our interpretation of $E(x_{AB})$ as a measure of the entanglement carried by $|x_{AB}\rangle$ is confirmed by this protocol as well.

The distillable entanglement and the entanglement cost are what called *operational measures of entanglement*, due to their origin. According to the previous arguments we can state the following:

Theorem 2.3. *For a pure bipartite state $|\psi\rangle$ the entropy of entanglement is equal to both the distillable entanglement and the entanglement cost of the state*

$$E(\psi) = E_D(\psi) = E_C(\psi) \tag{2.23}$$

Given its huge success, it is no wonder that the entropy of entanglement is considered as the unique measure of entanglement for pure bipartite states.

2.3 Concurrence and 2-tangle

The entropy of entanglement is a measure for pure bipartite systems of any size. However, when we focus on the simplest scenario of a two-qubit system, quantifying entanglement becomes remarkably more simple than calculating the system's entropy itself. The reduced density operator ρ_A of a qubit is represented by a 2×2 matrix. For such a matrix, we know the eigenvalues depend on its trace and its determinant. Since ρ_A has a unit trace, the determinant becomes the only remaining parameter. The characteristic equation of such a matrix is

$$\lambda^2 - (\mathrm{Tr}\,\rho_A)\,\lambda + \det\rho_A = 0 \implies \lambda^2 - \lambda + \det\rho_A = 0 \tag{2.24}$$

It can be shown that matrices with unit trace have the property

$$\det \rho_A = \frac{1}{2}\left(1 - \operatorname{Tr} \rho_A^2\right) \tag{2.25}$$

Here, we recognize a familiar quantity—the purity of a density matrix $\mathcal{P} = \operatorname{Tr} \rho_A^2$. In the first chapter we discussed how it can distinguish product states from entangled ones. As it turns out, it is also sufficient on its own to quantify the entanglement of qubits. In this context we introduce a "new" measure[4]:

Definition 2.4. *We define the* ***concurrence*** *of a pure state $|\psi\rangle$ of two qubits to be the quantity*

$$C(\psi) = 2\sqrt{\det \rho_A} = \sqrt{2\left(1 - \operatorname{Tr} \rho_A^2\right)} \tag{2.26}$$

The concurrence is a number in the range $[0, 1]$, vanishing for product states and reaching its maximum value of 1 for maximally entangled states. The above characteristic equation then becomes

$$\lambda^2 - \lambda + \det \rho_A = 0 \implies \lambda^2 - \lambda + \frac{1}{4}C^2 = 0 \tag{2.27}$$

The discriminant is $\Delta = 1 - C^2 \geq 0$ because $C \leq 1$, so there are always real roots. We can now easily determine the eigenvalues in terms of the concurrence, meaning we can express the entropy of entanglement as a function of the concurrence. We get

$$S(\rho_A) = \mathcal{E}(C) \tag{2.28}$$

with $\mathcal{E}$ being the function

$$\mathcal{E}(C) = -\frac{1 + \sqrt{1 - C^2}}{2} \log \frac{1 + \sqrt{1 - C^2}}{2} - \frac{1 - \sqrt{1 - C^2}}{2} \log \frac{1 - \sqrt{1 - C^2}}{2} \tag{2.29}$$

This is a monotonically increasing function that ranges from 0 to 1 as C goes from 0 to 1, meaning we can consider the concurrence as a measure of entanglement on its own. This monotonic relation between the entropy of entanglement and concurrence is plotted in Figure 2.1.

[4] We anticipate that any additional measure will not be original, but rather linked to the entropy of entanglement

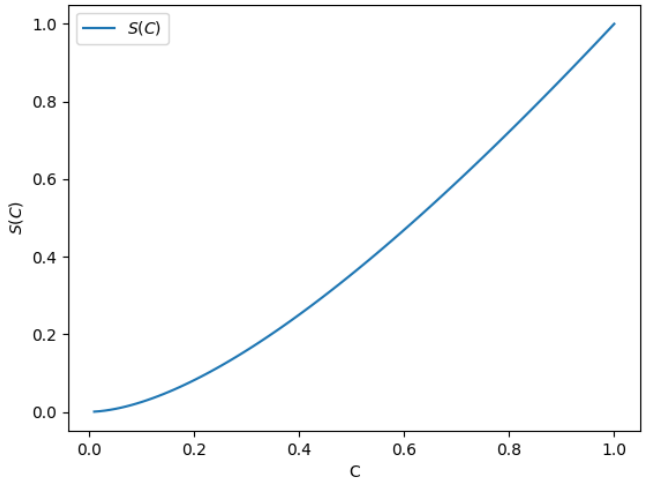

Figure 2.1: The von Neumann entropy as a function of concurrence for pure two-qubit states

Example

Let us consider a simple example to further illustrate the equivalence of these two measures. Suppose we have two interacting spin 1/2 particles A and B in the initial product state $|\psi(0)\rangle = |\uparrow\rangle_A |\downarrow\rangle_B$, with $\{|\uparrow\rangle, |\downarrow\rangle\}$ being the orthonormal eigenstates of the spin operator in the z-axis. The Hamiltonian describing the interaction is of the form

$$H_{int} = \frac{g}{\hbar^2}\vec{S}_A \cdot \vec{S}_B = \frac{g}{2\hbar^2}\left(S^2 - S_A^2 - S_B^2\right) \tag{2.30}$$

where $\vec{S}_A, \vec{S}_B$ are the individual spin operators and $\vec{S}$ is the total spin of the system AB. Since the system is in a pure state, the evolution in time is unitary. In order to compute the evolved state after time t, we express $|\psi(0)\rangle$ in terms of the eigenstates $|s, m_s\rangle$ of the total spin in the z-axis, S_z, using the Clebsch-Gordan coefficients: $|\psi(0)\rangle = (|0,0\rangle + |1,0\rangle)/\sqrt{2}$. We have

$$\begin{aligned} |\psi(t)\rangle &= U(t)\,|\psi(0)\rangle \\ &= \exp\left[-\frac{igt}{2\hbar^3}\left(S^2 - S_A^2 - S_B^2\right)\right]\frac{1}{\sqrt{2}}\left(|0,0\rangle + |1,0\rangle\right) \\ &= \cos\omega t\,|\uparrow\downarrow\rangle - i\sin\omega t\,|\downarrow\uparrow\rangle \end{aligned} \tag{2.31}$$

with $\omega = g/2\hbar$. In the last line we have neglected an overall phase $\exp(i\omega t/2)$, since it does not have any physical significance. If we next trace out the degrees of freedom of particle B, we are left with the density matrix

$$\rho_A = \begin{pmatrix} \cos^2\omega t & 0 \\ 0 & \sin^2\omega t \end{pmatrix} \tag{2.32}$$

From here we calculate the concurrence and the von Neumann entropy of this state

$$C(t) = |\sin 2\omega t| \quad \text{and} \quad S(t) = \mathcal{E}(|\sin 2\omega t|) \tag{2.33}$$

In Figure 2.2 we plot the values of these two measures over a period of $2\pi/\omega$. While they aren't exactly the same, they align for maximally entangled and product states. Additionally, they function equally effectively as measures of entanglement: when comparing any pair of states, they consistently identify the more entangled one.

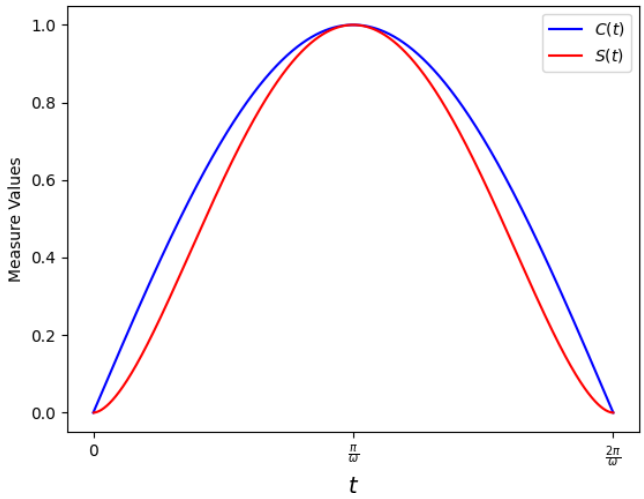

Figure 2.2: Entropy and concurrence for two interacting spin 1/2 particles

2-tangle: an easier alternative

To measure the degree of entanglement in a state using concurrence, one performs a partial trace operation and then calculates the determinant of the resulting density matrix. While this process is not complex for two-qubit systems, it can be simplified even further. To streamline this process, we'll adopt a slightly different approach, introducing another "new" measure that is easier to compute. Let's start by considering an arbitrary pure state of two qubits in the standard decomposition

$$|\psi_{AB}\rangle = \sum_{i_1,i_2=0}^{1} a_{i_1 i_2} |i_1 i_2\rangle \tag{2.34}$$

We organize the coefficients $a_{i_1 i_2}$ of the quantum state into the matrix:

$$A = (a_{i_1 i_2}) = \begin{pmatrix} a_{00} & a_{01} \\ a_{10} & a_{11} \end{pmatrix} \tag{2.35}$$

which we call the *coefficient matrix* of the state. By representing the coefficients in this particular way, we can state a simple condition for the factorization of the state

Theorem 2.5. *A pure state of two qubits is factorizable if and only if the determinant of the coefficient matrix vanishes:* $|\psi_{AB}\rangle = |\varphi_A\rangle \otimes |\chi_B\rangle \iff \det A = 0$

Proof For a product state, the coefficients can be factorized: $a_{i_1 i_2} = a_{i_1} a_{i_2}$, which immediately leads to $\det A = 0$. Conversely, if the determinant vanishes, either a column (or a row) of A is zero, indicating a product state, or the two columns are linearly dependent. Assuming $a_{01} = \lambda a_{00}$ and $a_{11} = \lambda a_{10}$ for some $\lambda \in \mathbb{C}$, we obtain:

$$
\begin{aligned}
|\psi\rangle &= a_{00}|00\rangle + a_{01}|01\rangle + a_{10}|10\rangle + a_{11}|11\rangle \\
&= a_{00}|0\rangle \otimes (|0\rangle + \lambda|1\rangle) + a_{10}|1\rangle \otimes (|0\rangle + \lambda|1\rangle) \\
&= (a_{00}|0\rangle + a_{10}|1\rangle) \otimes (|0\rangle + \lambda|1\rangle) \quad \blacksquare
\end{aligned} \tag{2.36}
$$

Hence, by examining the linear dependence between the two columns of A, we can readily determine whether a given state is entangled. Moreover, the modulus of the determinant achieves its maximum value of 1/2 for maximally entangled states such as the Bell states. Therefore, it is natural to define an entanglement measure based on this quantity:

Definition 2.6. *Consider a pure state $|\psi\rangle$ describing two qubits, with a corresponding coefficient matrix A. We define the* ***2-tangle*** *of the state as*

$$
\tau(\psi) = |\det A|^2 \tag{2.37}
$$

Next we will demonstrate that the 2-tangle is related to the concurrence, by bridging the gap between the description with density matrices and the one with the coefficient matrix. Let us evaluate the elements of the density matrix ρ_A in the general case

$$
\begin{aligned}
\rho_A &= \mathrm{Tr}_B |\psi\rangle\langle\psi| \\
&= \mathrm{Tr}_B \sum_{i_1,i_2} \sum_{j_1,j_2} a_{i_1 i_2} a^*_{j_1 j_2} |i_1 i_2\rangle\langle j_1 j_2| \\
&= \sum_{i_1,j_1} \sum_{k_2} a_{i_1 k_2} a^*_{j_1 k_2} |i_1\rangle\langle j_1|
\end{aligned} \tag{2.38}
$$

By simplifying the subscript names we can write

$$
(\rho_A)_{ij} = \sum_k a_{ik} a^*_{jk} = \sum_k A_{ik} A^\dagger_{kj} \tag{2.39}
$$

It is apparent that a matrix product has emerged:

$$
\rho_A = A A^\dagger \tag{2.40}
$$

By following the same steps for the other subsystem, we find that $\rho_B = A^T A^*$. We have thus found simple equations that relate the reduced density matrix of each subsystem with the coefficient matrix. That is exactly what we were looking for. It is worth noting that the above calculations are not specific to qubits, because the upper limit of these sums can be arbitrary. Therefore the same can be said for any bipartite system. As a consequence of these compact equations, and by using properties of the determinant, we obtain

$$
\det \rho_A = \det \rho_B = \det A A^\dagger = |\det A|^2 \implies \tau = \frac{1}{4} C^2 \tag{2.41}
$$

From this equation we conclude that the 2-tangle can indeed be used as a measure of entanglement, and works equally well as the concurrence, and by extension, the entanglement entropy.

Hence, in order to evaluate the amount of entanglement of a pure state, no partial trace is needed. All we have to do is observe the coefficients of the state, and calculate the determinant of A.

What can be said about higher level systems? Higher dimensions introduce extra parameters, and no simple analogue of (2.28) has been found. For example, it is a matter of algebra to show that the characteristic equation for a density matrix of a qutrit ($d = 3$) is

$$\lambda^3 - \lambda^2 + \left(\sum \tau_{2\times 2}\right)\lambda + \tau = 0 \tag{2.42}$$

Here, with $\tau_{2\times 2}$ we denote all the 2-tangles resulting from the possible 2×2 sub-determinants of the 3×3 coefficient matrix A, and τ has the usual definition (2.37). However, if the coefficient matrix is not of full rank, i.e. $\tau = 0$, then there exist at most two non-zero eigenvalues of the density matrix satisfying the equation

$$\lambda^2 - \lambda + \sum \tau_{2\times 2} = 0 \tag{2.43}$$

which is precisely the characteristic equation for qubits but with the sum $\sum \tau_{2\times 2}$ replacing the 2-tangle. The rank of the coefficient matrix A, or equivalently the Schmidt number of the reduced density matrix determines the entanglement structure of a bipartite system. We can say that for two n-dimensional qudits we find n different classes of entanglement: these correspond to values of the Schmidt number ranging from $K = 1$ (product state), $K = 2$ (qubit-like), all the way to $K = n$.

Chapter 3

Mixed State Entanglement

In accordance with the definition provided in Chapter 1, a mixed bipartite state ρ_{AB} is called separable if it can be expressed as a convex sum of product states. If such a decomposition impossible, the state is entangled. Our objective is to extend the existing tools of measuring entanglement to include mixed states. We can rule out the von Neumann entropy of one subsystem, because a basic requirement of entanglement measures is no longer met: separable states, that contain no entanglement, can have a non-zero value of entropy

$$\rho_A = \mathrm{Tr}_B \rho_{AB} = \sum_i p_i \rho_i^A \implies S(\rho_A) \neq 0 \text{ in general} \tag{3.1}$$

Therefore the von Neumann entropy fails to distinguish classical from quantum correlations for mixed states. Given that this metric is essentially the only tool for pure states, we need to go back to the drawing board. The von Neumann entropy was established as an operational entanglement measure through the distillation and dilution protocols. Is there a way to manipulate those processes to accommodate mixed sates? One finds out that entanglement distillation runs into an obstacle; it is possible that an entangled mixed state has zero distillable entanglement, meaning its entanglement cannot be used to extract a collection of Bell pairs. We say that these states contain *bound entanglement*. Therefore, unlike pure states, the creation of entangled mixed states is irreversible. This irreversibility is expected, since creating a mixed state from a pure state involves discarding some information.

3.1 Entanglement of Formation

We will attempt to generalize the dilution protocol, following a line of reasoning similar with the pure case. Our two observers, Alice and Bob, initially share many copies of Bell states, and they want to produce copies of a specific mixed state ρ. They are allowed no quantum communication, but only LOCC. Our goal is to compute the number of Bell states that have to be spent, asymptotically, for each copy of the state ρ created. We begin by taking the decomposition of ρ into pure states

$$\rho = \sum_i p_i |\varphi_i\rangle \langle\varphi_i| \tag{3.2}$$

with the set $\{|\varphi_i\rangle\}$ not necessarily being orthogonal. Following the protocol for pure states, Alice and Bob can create np_i copies of each state of the above decomposition, and this process will have cost them (asymptotically) $np_iE(\varphi_i)$ Bell states. This way they produce a total of n pairs, which they then collect into a large ensemble. They final step is to remove any trace that might help them associate a state with a particular pair of particles. In the end they find themselves with a collection of pairs, where each pair could be in any of the states $|\varphi_i\rangle$ with

probability p_i. In other words, each pair is now in the mixed state ρ. The total cost of this process is

$$n \sum_i p_i E(\varphi_i) \tag{3.3}$$

number of Bell states. This number is obviously dependent on the particular decomposition that was chosen in (3.2). But no physical property should depend on such choice. If we want to measure the minimum number of Bell states required to create ρ, we need to find the decomposition that minimizes the expression (3.3). Having said all of that, we present an entanglement measure for mixed bipartite states

Definition 3.1. *We define the* ***entanglement of formation*** *of a mixed state ρ as*

$$E_f(\rho) = \min \sum_i p_i E(\varphi_i) \tag{3.4}$$

with the minimum taken over all decompositions of ρ into pure states. This is what we call the *convex roof extension* of a pure-state measure into mixed states. In contrast with distillable entanglement, the above expression vanishes if and only if the state is separable. Monotonicity of the entanglement of formation has also been demonstrated in [10], meaning $E_f(\rho)$ meets the requirements of entanglement measures. That is something we expected, because if a measure is monotone on pure states, then we know its convex roof extension is monotonous on mixed states.

However, there are a couple of things that must be mentioned. First, the dilution process that we described is *approximate*. The physical pairs we created will not always be in the state ρ, but rather in approximations of it. For instance, if p_i is irrational, then we can never make exactly np_i copies of the pure state $|\varphi_i\rangle$ with finite n. We can, nonetheless, produce a state with arbitrarily good fidelity to the desired one, as long as n approaches infinity. The second, more interesting comment, is related to the so-called "additivity question", and whether E_f is indeed equal to the entanglement cost E_C for mixed states.

We showed that entanglement of formation quantifies the quantum resources needed, in terms of Bell states, to produce an ensemble of pure states representing a particular mixed state ρ. But is it the same as creating many copies of ρ itself? Let us think of it this way. Our goal is to create a large number of n copies of the state ρ, and for the sake of argument, we assume that n is even. Then, our task is the same as making $n/2$ copies of the state $\rho \otimes \rho$. Instead of decomposing ρ into pure states, we can express the tensor product $\rho \otimes \rho$ as a mixture of pure states of the larger Hilbert space. Following the standard dilution protocol, we can create these pure states from maximally entangled ones. Is there any advantage in following this alternative route? Are fewer Bell states required? Essentially we want to find out if $E_f(\rho \otimes \rho)$ is equal to $2E_f(\rho)$, or more generally, if $E_f(\rho^{\otimes N})$ is equal to $NE_f(\rho)$. This is known as the *additivity* question. If there is an advantage in treating many pairs together as a unit, meaning $E_f(\rho^{\otimes N}) < NE_f(\rho)$, then the entanglement of formation does not represent the entanglement cost for the creation of a single copy of ρ. In this case, one would want to look at the *regularized entanglement of formation*, defined as

$$E_f^{\infty}(\rho) = \lim_{N\to\infty} \frac{E_f(\rho^{\otimes N})}{N} \tag{3.5}$$

In [11] it was proven that this limit exists, and furthermore, it is the most efficient way of creating many copies of ρ. In other words, the entanglement cost is equal to the regularized entanglement of formation. For a long time it was not known whether this is the same as the entanglement of formation, namely, if the latter is additive. Examples of states with additive E_f have been found. For example, it has been shown that for any state of the form

$$\rho = \sum_{i,j} a_{ij} |ii\rangle \langle jj| \tag{3.6}$$

E_f is additive [6]. Later, a statement equivalent to the additivity of the entanglement of formation was proven false by [12], meaning the entanglement of formation is not equal to the entanglement cost.

Concurrence

The entanglement of formation is admittedly quite abstract, as per the fact that it requires a minimization over all pure-state decompositions. It would be incredibly useful if we had an exact formula, which given an arbitrary state ρ, can be used to quantify its entanglement. We recall that for qubits the entropy of entanglement can be expressed as a monotonically increasing function of a quantity that we named concurrence

$$E(\psi) = \mathcal{E}(C(\psi)) \tag{3.7}$$

We defined the concurrence through the determinant of the density matrix of one subsystem. An alternative definition could be

$$C = \left|\langle\psi|\tilde{\psi}\rangle\right| \tag{3.8}$$

where $|\tilde{\psi}\rangle$ is the "spin-flip" state

$$|\tilde{\psi}\rangle = \left(\sigma_y \otimes \sigma_y\right) |\psi\rangle^* \tag{3.9}$$

with σ_y being the Pauli matrix and $|\psi\rangle^*$ the complex conjugate of $|\psi\rangle$ in the standard basis. One can take the general form of a pure state $|\psi\rangle$ and easily verify that the expression (3.8) agrees with the original definition of the concurrence in (2.26). The spin-flip operation, when applied to a pure product state, reverses the direction of the spin for each qubit. Visually, this operation takes each state to its diametrical opposite on the Bloch sphere. As a consequence of projecting a product state to its orthogonal, the concurrence of such a state is zero. When it comes to the other extreme, completely entangled states are left, up to an overall phase, unchanged by the spin-flip. Thus, their concurrence takes the maximum value of one.

But why are we mentioning all this? The reason is that, fortunately, the formula (3.7) can be extended to the entanglement of formation without any modification. Wootters [13] showed how to construct entanglement-minimizing pure-state decompositions for two qubits, providing an explicit formula for the entanglement of formation. The result is the following:

Theorem 3.2. *The entanglement of formation E_f of an arbitrary mixed state ρ describing a two-qubit system can be expressed as*

$$E_f(\rho) = \mathcal{E}(C(\rho)) \tag{3.10}$$

with $\mathcal{E}$ being our familiar function from (2.29), and $C(\rho)$ denoting the ***concurrence*** *of mixed states, defined as a convex roof extension*

$$C(\rho) = \min_{\varphi_i} \sum_i p_i C(\varphi_i) \tag{3.11}$$

Again, the minimum is taken over all pure-state decompositions of ρ. The closed form of the concurrence is given by

$$C(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\} \tag{3.12}$$

Here, the λ_i are the eigenvalues, in decreasing order, of the Hermitian operator

$$R = \sqrt{\sqrt{\rho}\,\tilde{\rho}\,\sqrt{\rho}} \tag{3.13}$$

and they are real, non-negative numbers. With $\tilde{\rho}$ we denote the generalization of the spin-flip operation for density matrices

$$\tilde{\rho} = \left(\sigma_y \otimes \sigma_y\right) \rho^* \left(\sigma_y \otimes \sigma_y\right) \tag{3.14}$$

Alternatively, the λ_i may be calculated as the square roots of the eigenvalues of the non-Hermitian matrix $\rho\tilde{\rho}$. The above formula for the concurrence, although being a bit strange, reduces to the known expression for pure states. It will prove to be particularly useful when we will discuss the entanglement of three qubits, and particularly, how it is distributed between the three parties.

3.2 Geometric Measures: Relative Entropy of Entanglement

Thus far we have remained faithful to operational measures of entanglement, and given their clear physical interpretation, it comes as no surprise. But this is by no means the only approach to quantifying entanglement. Another school of thought involves constructing *geometric* entanglement measures. The basic premise is quite simple: for an arbitrary entangled state we want to find its closest separable state. But what do we mean by 'closest'? We need to know how to measure the distance between two density matrices. If we agree on such a measure measure of distance D, we can then define a measure of entanglement for an arbitrary bipartite state σ to be

$$E(\sigma) = \min_{\rho \in \mathcal{D}} D(\sigma \| \rho) = D(\sigma \| \rho^*) \tag{3.15}$$

where $\mathcal{D}$ represents the set of all disentangled (separable) states, and ρ^* is the state that minimizes the chosen distance. There is no reason to restrict our candidates for a distance D only to metrics, but we certainly ask that our choice is consistent with the requirements for $E(\sigma)$ as an entanglement measure. A geometric measure (3.15) attempts to quantify only the quantum part of the correlations existing in a state σ, that originate from entanglement. Therefore all remaining correlations in its closest disentangled state ρ^* must be classical in nature. Following the same recipe, one can search for the closest uncorrelated state to ρ^*, and the corresponding distance could be interpreted as a measure of the classical correlations present in σ.

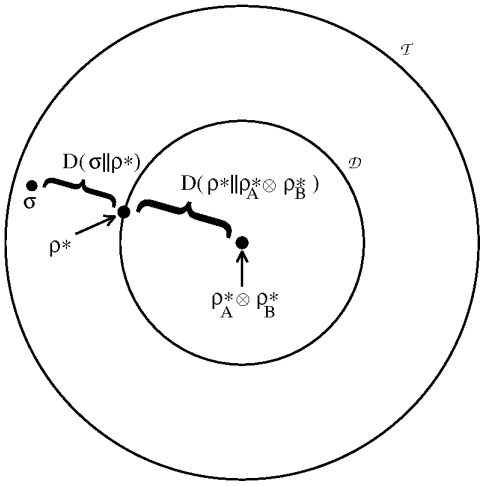

Figure 3.1: A visual representation of the set $\mathcal{T}$ of all density matrices. A subset $\mathcal{D}$ of $\mathcal{T}$ contains all disentangled states, and for every entangled state $\sigma \in \mathcal{T} \setminus \mathcal{D}$ we denote with ρ^* its closest disentangled state with respect to a measure of distance $D(\sigma||\rho)$. The distance $D\left(\rho^* \| \rho_A^* \otimes \rho_B^*\right)$ where ρ_A and ρ_B are obtained by tracing over the subsystems, quantifies the classical part of the correlations in σ.

Let us address the first issue: what will be our chosen measure of distance? From all the candidates that have been proposed, one seems to stand out: the *relative entropy*, defined as

$$S(\sigma \| \rho) = \operatorname{Tr} \sigma (\log \sigma - \log \rho) \tag{3.16}$$

This is the quantum analog of the Kullback–Leibler divergence in statistics. Given two probability distributions of a finite sequence of events $P = \{p_1, \ldots, p_n\}$ and $Q = \{q_1, \ldots, q_n\}$, the K-L divergence is defined as

$$D_{KL}(P \| Q) = \sum_{i=1}^{n} p_i \log p_i - \sum_{i=1}^{n} p_i \log q_i \tag{3.17}$$

It is a kind of statistical distance, measuring how distinguishable the distribution P is from a reference distribution Q. It can be interpreted as the error we will make in predicting the uncertainty of these random events if we assume the probability distribution is P, but in reality it is Q. Likewise, it can be said that the relative entropy measures the distinguishability of two density matrices. Having established a measure of distance, we are now in a position to present the resulting entanglement measure according to (3.15).

Definition 3.3. *For a mixed quantum state σ we define the* ***relative entropy of entanglement (REE)*** *to be*

$$E_R(\sigma) = \min_{\rho \in \mathcal{D}} S(\sigma \| \rho) = S(\sigma \| \rho^*) \tag{3.18}$$

Higher values of REE imply greater departure from seperability, and conversely, a lower REE suggests that the state σ can be closely approximated by a separable state, signifying weaker entanglement. As one might notice right away from the definition (3.16) the relative entropy is not symmetric in its arguments. Nor does it satisfy the triangle inequality. It is therefore not a true metric, but rather, a quasidistance. So why do we insist on using the relative entropy to measure the distance of density matrices? To begin with, the REE meets all the

requirements of entanglement measures. It is a non-negative quantity that vanishes if and only if the input state is separable. Furthermore it is LU invariant and non-increasing under LOCC. But the most important reason is that the REE of pure states coincides with their entropy of entanglement, and to our knowledge, REE is the only geometric measure to do so. This property is very desirable, to an extent that some view it as an additional condition for measures of entanglement. Let us demonstrate these properties one at a time.

Theorem 3.4. *For any two density matrices σ, ρ their relative entropy is non-negative*

$$S(\sigma \| \rho) \geq 0 \tag{3.19}$$

with the equality holding if and only if $\sigma = \rho$.

Proof We will use the spectral decompositions of these matrices

$$\sigma = \sum_i p_i |u_i\rangle \langle u_i| \quad \text{and} \quad \rho = \sum_i q_i |w_i\rangle \langle w_i| \tag{3.20}$$

and substitute them in (3.16) to directly calculate the relative entropy. The first term is straightforward to compute since the matrix $\rho \log \rho$ is diagonal in the basis $\{|u_i\rangle\}$. The second term needs some work done. We have

$$\begin{aligned} S(\sigma \| \rho) &= \operatorname{Tr} \sigma \log \sigma - \operatorname{Tr} \sigma \log \rho \\ &= \sum_i p_i \log p_i - \operatorname{Tr} \left(\sum_i p_i |u_i\rangle \langle u_i| \right) \left(\sum_j \log q_j |w_j\rangle \langle w_j| \right) \\ &= \sum_i p_i \log p_i - \sum_{i,j} \left| \langle u_i | w_j \rangle \right|^2 p_i \log q_j \\ &= \sum_i p_i \left(\log p_i - \sum_j P_{ij} \log q_j \right) \end{aligned} \tag{3.21}$$

with $P_{ij} = \left| \langle u_i | w_j \rangle \right|^2$ matrix elements that satisfy $\sum_i P_{ij} = \sum_i P_{ij} = 1$. Because $-\log x$ is a convex function, Jensen's inequality applies, which gives

$$-\sum_j P_{ij} \log q_j \geq -\log \left(\sum_j P_{ij} q_j \right) \tag{3.22}$$

The numbers $r_i = \sum_j P_{ij} q_j$ can be considered as a probability distribution, because

$$\sum_i r_i = \sum_{i,j} P_{ij} q_j = \sum_j q_j = \operatorname{Tr} \sigma = 1 \tag{3.23}$$

Keeping that in mind, we have found that the relative entropy satisfies

$$S(\sigma \| \rho) \geq \sum_i p_i (\log p_i - \log r_i) = \sum p_i \left(-\log \frac{r_i}{p_i} \right) \tag{3.24}$$

By applying Jensen's inequality one more time we finally obtain

$$S(\sigma\|\rho) \geq -\log\left(\sum_i p_i \frac{r_i}{p_i}\right) = -\log\sum_i r_i = 0 \tag{3.25}$$

The case of equality is achieved in (3.22) if and only if P_{ij} is a permutation matrix. Given the definition of these numbers, and proper renaming of the eigenstates $\{|u_i\rangle\},\{|v_i\rangle\}$, this implies that $\sigma = \rho$. ■

As the relative entropy is a form of trace distance, it is naturally invariant under local unitary transformations, and this inherent invariance extends to the REE. Additionally, it was shown by Lindblad [14] that the relative entropy is monotonically decreasing under any completely positive trace preserving (CPTP) operation $\mathcal{N}$ on density matrices

$$S(\mathcal{N}\sigma\|\mathcal{N}\rho) \leq S(\sigma\|\rho) \tag{3.26}$$

The implication is that REE also exhibits this behavior. If ρ^* is the state that realizes the minimum of (3.18), then

$$E_R(\sigma) = S(\sigma\|\rho^*) \geq S(\mathcal{N}\sigma\|\mathcal{N}\rho^*) \geq \min_{\rho\in\mathcal{D}} S(\mathcal{N}\sigma\|\rho) = E_R(\mathcal{N}\sigma) \tag{3.27}$$

Considering that LOCC are a subset of CPTP operations, this argument proves the monotonicity of REE.

Theorem 3.5. *For an arbitrary pure two-qubit state σ, its relative entropy of entanglement is equal to its entropy of entanglement, which is simply the von Neumann entropy of one subsystem.*

Proof Let $\sigma = |\psi\rangle\langle\psi|$ be a pure state of two qubits, with $|\psi\rangle$ expressed in the Schmidt decomposition as $|\psi\rangle = \sqrt{p}\,|00\rangle + \sqrt{1-p}\,|11\rangle\langle 11|$. Let us also consider the disentangled state $\rho = p\,|00\rangle\langle 00| + (1-p)\,|11\rangle\langle 11|$. First we will prove that the relative entropy $S(\sigma\|\rho)$ is equal to the entropy of entanglement of σ. Then we will establish that ρ is actually the closest disentangled state to σ, since it minimizes the relative entropy.

$$\begin{aligned}
S(\sigma\|\rho) &= \cancelto{0}{\operatorname{Tr}\sigma\log\sigma} - \operatorname{Tr}\sigma\log\rho \\
&= -\operatorname{Tr}\left\{\left(\sqrt{p}\,|00\rangle + \sqrt{1-p}\,|11\rangle\right)\left(\sqrt{p}\,\langle 00| + \sqrt{1-p}\,\langle 11|\right)\left(\log p\,|00\rangle\langle 00| + \log(1-p)\,|11\rangle\langle 11|\right)\right\} \\
&= -\operatorname{Tr}\Big\{p\log p\,|00\rangle\langle 00| + \sqrt{p(1-p)}\log(1-p)\,|00\rangle\langle 11| + \sqrt{p(1-p)}\log p\,|11\rangle\langle 00| \\
&\qquad + (1-p)\log(1-p)\,|11\rangle\langle 11|\Big\} \\
&= -p\log p - (1-p)\log(1-p) \\
&= E(\sigma)
\end{aligned} \tag{3.28}$$

Now assume that we make a small change in ρ, getting the state

$$\rho_\lambda = (1-\lambda)\rho + \lambda\rho^* \tag{3.29}$$

for some small λ such that ρ_λ and ρ^* are disentangled. For ρ to minimize the relative entropy, it must be true that

$$\frac{d}{d\lambda} S\left(\sigma \| \rho_\lambda\right)\Big|_{\lambda=0} \geq 0 \tag{3.30}$$

Because the relative entropy is a convex on its second argument, this condition with the first derivative is sufficient to establish that ρ minimizes the function. In the following demonstration we will employ the representation of the logarithm of a density operator through integration in the complex plane. We can write

$$\log \rho = \frac{1}{2\pi i} \oint dz \log z \frac{1}{zI - \rho} \tag{3.31}$$

where the contour of integration encloses all the eigenvalues of the matrix ρ. Since we are only interested in the sign of the derivative in (3.30), our argument is not affected by a change of basis in the logarithm, because it only produces a scaling factor. Thus, for the rest of this proof, we will be using the natural logarithm in order to avoid carrying a scaling factor of $1/\ln 2$. With that being said, we have

$$\begin{aligned}
\frac{d}{d\lambda} S\left(\sigma \| \rho_\lambda\right)\Big|_{\lambda=0} &= -\frac{d}{d\lambda} \operatorname{Tr}\left\{\sigma \rho_\lambda\right\}\Big|_{\lambda=0} \\
&= -\frac{d}{d\lambda} \operatorname{Tr}\left\{\sigma \frac{1}{2\pi i} \oint dz \, \frac{1}{zI - \rho_\lambda} \ln z\right\}\Big|_{\lambda=0} \\
&= -\frac{1}{2\pi i} \operatorname{Tr}\left\{\oint dz \left(\rho^* - \rho\right)(zI - \rho)^{-1} \sigma (zI - \rho)^{-1} \ln z\right\}
\end{aligned} \tag{3.32}$$

Since ρ is diagonal it is not difficult to compute the operators inside the integral. We obtain

$$\begin{aligned}
\rho (zI - \rho)^{-1} \sigma (zI - \rho)^{-1} =& \frac{p^2}{(z-p)^2} |00\rangle\langle 00| + \frac{(1-p)^2}{(z-1+p)^2} |11\rangle\langle 11| \\
&+ \frac{\sqrt{p(1-p)}}{(z-p)(z-1+p)} \left(p |00\rangle\langle 11| + (1-p) |11\rangle\langle 00|\right)
\end{aligned} \tag{3.33}$$

Because of the trace, the off-diagonal terms do not contribute to the calculations. Therefore, using Cauchy's theorem for complex integration we get

$$\begin{aligned}
I_1 &= \frac{1}{2\pi i} \operatorname{Tr}\left\{\oint dz \rho (zI - \rho)^{-1} \sigma (zI - \rho)^{-1} \ln z\right\} \\
&= \frac{1}{2\pi i} \oint dz \left\{p^2 \frac{\ln z}{(z-p)^2} + (1-p)^2 \frac{\ln z}{(z-1+p)^2}\right\} \\
&= p + 1 - p = 1
\end{aligned} \tag{3.34}$$

Similarly

$$\rho^* (zI-\rho)^{-1}\sigma(zI-\rho)^{-1} = \rho^*\left\{\frac{p}{(z-p)^2}|00\rangle\langle 00| + \frac{1-p}{(z-1+p)^2}|11\rangle\langle 11|\right.$$
$$\left. + \frac{\sqrt{p(1-p)}}{1-2p}\left(\frac{1}{z-1+p}-\frac{1}{z-p}\right)(|00\rangle\langle 11| + |11\rangle\langle 00|)\right\} \tag{3.35}$$

And

$$I_2 = \frac{1}{2\pi i}\mathrm{Tr}\left\{\oint dz\rho^*(zI-\rho)^{-1}\sigma(zI-\rho)^{-1}\ln z\right\}$$
$$= \ldots \tag{3.36}$$
$$= \mathrm{Tr}\{\rho^*[|00\rangle\langle 00| + |11\rangle\langle 11| + x(|00\rangle\langle 11| + |11\rangle\langle 00|)]\} \tag{3.37}$$

with

$$x = \frac{\sqrt{p(1-p)}[(\ln p - \ln(1-p)]}{2p-1} \tag{3.38}$$

From these results we arrive at

$$\frac{d}{d\lambda}S(\sigma\|\rho_\lambda)\Big|_{\lambda=0} = I_1 - I_2$$
$$= 1 - \mathrm{Tr}\{\rho^*[|00\rangle\langle 00| + |11\rangle\langle 11| + x(|00\rangle\langle 11| + |11\rangle\langle 00|)]\} \tag{3.39}$$

It can be verified that $x \leq 1$ with the maximum achieved for $p = 1/2$. Our derivative takes its minimum value for $x = 1$, meaning for it to be positive, it is sufficient to show that

$$\mathrm{Tr}\{\rho^*(|00\rangle\langle 00| + |11\rangle\langle 11| + |00\rangle\langle 11| + |11\rangle\langle 00|)\} \leq 1 \tag{3.40}$$

But it turns out this trace is equal to twice the overlap of ρ^* with the Bell state $|\Phi^+\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$

$$\mathrm{Tr}\{\rho^*(|00\rangle\langle 00| + |11\rangle\langle 11| + |00\rangle\langle 11| + |11\rangle\langle 00|)\} = 2\langle\Phi^+|\rho^*|\Phi^+\rangle \tag{3.41}$$

For separable states of two qubits such as ρ^*, the maximum overlap with completely entangled states, which is known as the *fidelity* F, is given by $F = 1/2$. When combined with the above result, this concludes our proof. It should be mentioned that although we presented the proof for two qubits, it can be easily extended to arbitrarily large subsystems. ■

Thus far in this chapter we have discussed two entanglement measures that are representatives of two different approaches to quantifying entanglement. Let us now try to compare them.

Theorem 3.6. *For any bipartite state σ, the entanglement of formation E_f and the REE E_R satisfy the relation*

$$E_f(\sigma) \geq E_R(\sigma) \tag{3.42}$$

Proof For the state σ there is by definition a pure-state decomposition $\sigma = \sum_i p_i \sigma_i$ such that $E_f(\sigma) = \sum_i p_i E_f(\sigma_i)$. But we know that for pure states, both the measures we are comparing coincide with the entropy of entanglement E. Therefore

$$E_f(\sigma) = \sum_i p_i E_f(\sigma_i) = \sum_i p_i E_R(\sigma_i) \geq E_R\left(\sum_i p_i \sigma_i\right) = E_R(\sigma) \tag{3.43}$$

Here we employed the convexivity of REE, a property held by good entanglement measures. It follows from the fact that the relative entropy is convex in both arguments, meaning

$$S(x_1\sigma_1 + x_2\sigma_2 \| x_1\rho_1 + x_2\rho_2) \leq x_1 S(\sigma_1\|\rho_1) + x_2 S(\sigma_2\|\rho_2) \tag{3.44}$$

for $x_1, x_2 \in [0,1]$ satisfying $x_1 + x_2 = 1$. If we denote with ρ_1^*, ρ_2^* the separable states closest to σ_1 and σ_2 respectively, we have

$$\begin{aligned} E_R(x_1\sigma_1 + x_2\sigma_2) &\leq S(x_1\sigma_1 + x_2\sigma_2 \| x_1\rho_1^* + x_2\rho_2^*) \\ &\leq x_1 S(\sigma_1\|\rho_1^*) + x_2 S(\sigma_2\|\rho_2^*) \\ &= x_1 E_R(\sigma_1) + x_2 E_R(\sigma_2) \quad \blacksquare \end{aligned} \tag{3.45}$$

3.3 PPT Criterion

In this section, we shift our focus from methods of quantifying entanglement to just answering a more fundamental question: does the quantum state exhibit any entanglement? Determining whether a state is separable or not is known as the separability problem in quantum information theory, and it is admittedly a challenging task. In 1996 Peres [16] and the Horodecki family [17] presented a criterion for seperability of bipartite quantum states. Establishing this criterion requires a familiarity with the notion of the partial transpose of a density matrix. A bipartite state ρ can be written in terms of the basis vectors of the individual subsystems as

$$\rho = \sum_{i,j}\sum_{k,l} p_{ijkl} |i_A\rangle\langle j_A| \otimes |k_B\rangle\langle l_B| \tag{3.46}$$

In the Dirac formalism, the transpose of an operator is obtained by interchanging the kets and bras of the basis states. By applying this transformation to just one subsystem we get the *partial transpose operator*

$$\rho^{T_B} = (I_A \otimes T_B)\rho = \sum_{i,j}\sum_{k,l} p_{ijkl} |i_A\rangle\langle j_A| \otimes |l_B\rangle\langle k_B| \tag{3.47}$$

Taking the partial transpose generally affects the eigenvalues of an operator, in such a way that positivity -a property held by all density matrices- might not be retained. As it turns out, this is is closely related to whether the initial state is entangled or not. What we know thus far can be summarized in the following criterion.

Theorem 3.7. *(PPT Criterion) Consider a bipartite system in a state ρ. If the partial transpose ρ^{T_B} has a negative eigenvalue, then ρ is entangled. Hence a positive partial transpose is a necessary condition for a density operator to be separable. For the special cases of 2×2 and 2×3 dimensional systems, the converse is also true, making the positivity of the partial transpose also a sufficient condition.*

Instead of presenting the full proof, we will take a shortcut and just verify that separable states maintain positivity of the partial transpose operator. By definition such states can be expressed as a convex combination of product states

$$\rho = \sum_i p_i \rho_i^A \otimes \rho_i^B \tag{3.48}$$

The partial transpose operation does not change the eigenvalues of a product state, and since these are always non-negative, the same is true for the eigenvalues of the partial transpose of ρ.

In the next section we apply everything we presented to study the entanglement of a particular family of mixed quantum states.

3.4 Bell-Diagonal States

Usually we express quantum states of two qubits (pure or mixed) in the computational basis. An alternative choice of basis is the set of the maximally entangled Bell states

$$\begin{aligned} |e_1\rangle = |\varphi^+\rangle &= \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \\ |e_2\rangle = |\varphi^-\rangle &= \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle) \\ |e_3\rangle = |\psi^+\rangle &= \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) \\ |e_4\rangle = |\psi^-\rangle &= \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle) \end{aligned} \tag{3.49}$$

The decomposition of an arbitrary mixed state ρ in the above basis takes the form

$$\rho = \sum_{i,j=1}^{4} p_{ij} |e_i\rangle \langle e_j| \tag{3.50}$$

This particular choice is very helpful in defining an important subset of two-qubit states that are referred to as *Bell-diagonal states*. These are density matrices that have a diagonal form in the Bell basis, i.e. we can write

$$\rho = \sum_{i=1}^{4} p_i |e_i\rangle \langle e_i|, \qquad \text{with} \quad \sum_{i=1}^{4} p_i = 1 \tag{3.51}$$

Each state within this set is entirely specified by just three independent parameters. This concise parameterization aids in both theoretical investigations and practical applications. Specifically, in the context of our study, the simplicity of Bell-diagonal states provides clarity in describing their entanglement properties. We will demonstrate that the application of the PPT criterion is straightforward, providing a clear and simple condition for determining separability. Additionally, we will discover precise formulas for the mixed-state entanglement measures that we previously introduced.

Theorem 3.8. *A Bell-diagonal state of two qubits in the form of (3.51) is separable if none of the probabilities exceed 1/2, i.e. if $p_i \leq 1/2$ for all four values of i.*

Proof The proof is a direct application of the PPT criterion, which as we know, determines the necessary and sufficient condition for separability of 2×2 systems. The effect of the partial transpose operation on each operator in the sum (3.51) is easily calculated if we switch back to the computational basis. For example

$$\begin{aligned}(I_A \otimes T_B)\left|\varphi^+\right\rangle\left\langle\varphi^+\right| &= (I_A \otimes T_B)\frac{1}{2}(|00\rangle + |11\rangle)(\langle 00| + \langle 11|) \\ &= (I_A \otimes T_B)\frac{1}{2}(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|) \\ &= \frac{1}{2}(|00\rangle\langle 00| + |01\rangle\langle 10| + |10\rangle\langle 01| + |11\rangle\langle 11|) \end{aligned} \tag{3.52}$$

The resulting partial transpose operator is represented in the computational basis by the matrix

$$\rho^{T_B} = \frac{1}{2}\begin{pmatrix} p_1 + p_2 & 0 & 0 & p_3 - p_4 \\ 0 & p_3 + p_4 & p_1 - p_2 & 0 \\ 0 & p_1 - p_2 & p_3 + p_4 & 0 \\ p_3 - p_4 & 0 & 0 & p_1 + p_2 \end{pmatrix} \tag{3.53}$$

After some algebra we find that the characteristic equation takes the form

$$\det\left(\rho^{T_B} - \lambda I\right) = 0 \implies \left[(p_1 + p_2 - 2\lambda)^2 - (p_3 - p_4)^2\right]\left[(p_3 + p_4 - 2\lambda)^2 - (p_1 - p_2)^2\right] = 0 \tag{3.54}$$

Which, combined with the condition $\sum_i p_i = 1$ yields

$$\lambda_i = \frac{1 - 2p_i}{2} \tag{3.55}$$

According to the PPT criterion separable states satisfy $\lambda_i \geq 0 \implies p_i \leq 1/2$. ■

Another desirable aspect of Bell-diagonal states is they allow for an exact solution to the minimization problem associated with the relative entropy of entanglement. It is also straightforward to calculate the entanglement of formation for these states. The results of these calculations are stated in the next theorem.

Theorem 3.9. *Consider a Bell-diagonal state $\sigma = \sum_{i=1}^4 p_i |e_i\rangle\langle e_i|$ that is entangled, meaning one of the probabilities satisfies $p_{max} \geq 1/2$. Then the relative entropy of entanglement for that state is given by*

$$E_R(\sigma) = 1 + p_{max}\log p_{max} + (1 - p_{max})\log(1 - p_{max}) = 1 - h(p_{max}) \tag{3.56}$$

with $h(x) = -x\log x - (1-x)\log(1-x)$ being the binary entropy function. The entanglement of formation of the state is given by

$$E_f(\sigma) = \mathcal{E}(2p_{max} - 1) \tag{3.57}$$

Proof From the definition of the relative entropy of entanglement we obtain

$$\begin{aligned} E_R(\sigma) &= \min_{\rho\in\mathcal{D}} \operatorname{Tr}(\sigma\log\sigma - \sigma\log\rho) \\ &= \sum_i p_i \log p_i + \min_{\rho\in\mathcal{D}} (-\operatorname{Tr}\sigma\log\rho) \\ &= \sum_i p_i \log p_i + \min_{\rho\in\mathcal{D}} \left(- \sum_i p_i \langle e_i|\log\rho|e_i\rangle \right) \end{aligned} \tag{3.58}$$

The next step in our proof involves using the spectral decomposition of ρ, the definition of the logarithm of a density matrix, as well as Jensen's inequality for the convex function $-\log x$. We obtain

$$E_R(\sigma) \geq \sum_i p_i \log p_i + \min_{\rho\in\mathcal{D}} \left(- \sum_i p_i \log \langle e_i|\rho|e_i\rangle \right) \tag{3.59}$$

Once again, we encounter the fidelity of a quantum state $F_i = \langle e_i|\rho|e_i\rangle$. Since ρ is a separable state, we know that $F_i \leq 1/2$ for all values of i. As a result, the problem at hand is equivalent to the following: we want to minimize the function $f(F_1, F_2, F_3, F_4) = -\sum_{i=1}^4 p_i \log F_i$ with the constraints $\sum_{i=1}^4 F_i = 1$ and $F_i \in [0, 1/2]$. We assume, without loss of generality, that the maximum probability in the initial state σ is $p_{max} = p_1$. Then the minimization yields

$$F_i = \begin{cases} 1/2, & i = 1 \\ \dfrac{p_i}{2(1-p_1)}, & i \neq 1 \end{cases} \tag{3.60}$$

Substituting these results to the REE formula we get

$$\begin{aligned} E_R(\sigma) &= \sum_{i=1}^4 p_i \log p_i - p_1 \log\frac{1}{2} - \sum_{i=2}^4 p_i \log\frac{p_i}{2(1-p_1)} \\ &= 1 + p_1 \log p_1 + (1-p_1)\log(1-p_1) \end{aligned} \tag{3.61}$$

which proves our first claim. We will now assess the entanglement of formation using the concurrence given by

$$C(\sigma) = \max\left\{0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}\right\} \tag{3.62}$$

where λ_i represents the eigenvalues, arranged in decreasing order, of the matrix $\sigma\tilde{\sigma}$. Here, $\tilde{\sigma}$ denotes the spin-flipped density matrix defined as $\tilde{\sigma} = \left(\sigma_y \otimes \sigma_y\right)\sigma\left(\sigma_y \otimes \sigma_y\right)$. The Kronecker product $\sigma_y \otimes \sigma_y$ is itself a Bell-diagonal matrix given by

$$\sigma_y \otimes \sigma_y = |\phi^-\rangle\langle\phi^-| - |\phi^+\rangle\langle\phi^+| + |\psi^+\rangle\langle\psi^+| - |\psi^-\rangle\langle\psi^-| \tag{3.63}$$

Hence this matrix commutes with any other Bell-diagonal state such as σ. This, coupled with the fact that $\left(\sigma_y \otimes \sigma_y\right)^2 = I$, implies that the spin-flip operation leaves any Bell-diagonal state unchanged. Therefore, $\sigma\tilde{\sigma} = \sigma^2$ and $\lambda_i = p_i^2$, meaning

$$
\begin{aligned}
C(\sigma) &= \max\left\{0, p_{max} - \sum_{i \neq \max} p_i\right\} \\
&= \max\{0, p_{max} - (1 - p_{max})\} \\
&= 2p_{max} - 1
\end{aligned} \tag{3.64}
$$

since for entangled states we showed that $p_{max} \geq 1/2$. As a result

$$
E_f(\sigma) = \mathcal{E}(2p_{max} - 1) \quad \blacksquare \tag{3.65}
$$

Having analytic expressions for these two measures allows us to plot their values in terms of the single parameter p_{max}, as seen in Figure 3.2, confirming that $E_f \geq E_R$.

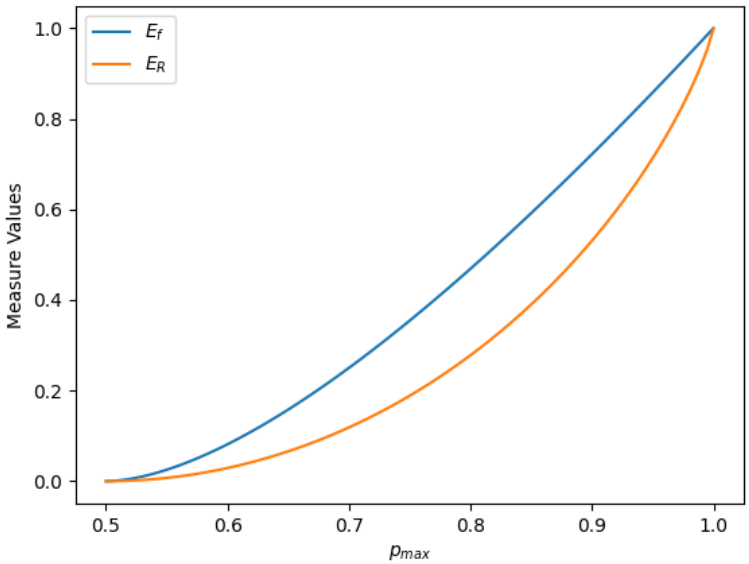

Figure 3.2: Joint plot of entanglement of formation and relative entropy of entanglement for Bell-diagonal states

Chapter 4

Tripartite Entanglement

In this chapter we will dive into the entanglement properties of systems with more than two parties, starting with the simplest generalization possible: a system composed of three qubits A,B and C. Even though we are only adding one qubit, the entanglement exhibits a much richer structure than bipartite systems, because there are several possible partitions of this larger system. As a result, the extension of already established descriptions of entanglement is anything but trivial. First we will study pure states of three qubits, generalizing the idea of the coefficient matrix and determining criteria for factorization. An entanglement measure emerges, called the 3-tangle, which quantifies genuine tripartite entanglement. We find out that entangled states can be split into two inequivalent classes, and members of each class can be converted into each other by means of stochastic local operations and classical communication (SLOCC). Lastly we take a look at some important entropy inequalities such as the strong subadditivity of quantum entropy (SSA).

4.1 Coefficient Hypermatrix and the 3-tangle

As we have established, it is the case for bipartite systems that the determinant, as well as the sub-determinants of the coefficient matrix A provide insight to the entanglement properties of pure states. It is only natural to search for a similar description for a system of three qubits. An arbitrary pure state of such a system can be expressed in the computational basis as

$$|\psi\rangle = \sum_{i_1,i_2,i_3=0}^{1} a_{i_1 i_2 i_3} |i_1 i_2 i_3\rangle \tag{4.1}$$

What is the generalization of the coefficient matrix? In other words, what algebraic object is better fit to represent the 8 coefficients $a_{i_1 i_2 i_3}$? In order to capture the tripartite nature of the quantum state, we choose the $2 \times 2 \times 2$ hypermatrix A

$$A = (a_{i_1 i_2 i_3}) \tag{4.2}$$

It is evident in the structure shown in Figure 4.1 that we have associated each qubit with one coordinate axis in $\mathbb{R}^3$, in the sense that, for example, the face of the hypermatrix that lies in the plane $x = 0$ contains only coefficients of states where qubit A takes the value 0. We thus define the six submatrices

$$
\begin{aligned}
A_{x_0} &= (a_{0i_2i_3}), \quad A_{x_1} = (a_{1i_2i_3}) \\
A_{y_0} &= (a_{i_10i_3}), \quad A_{y_1} = (a_{i_11i_3}) \\
A_{z_0} &= (a_{i_1i_20}), \quad A_{z_1} = (a_{i_1i_21})
\end{aligned} \tag{4.3}
$$

which on their own play a significant role in determining some entanglement properties of the quantum state, leading to factorization conditions, as it will be shown later on.

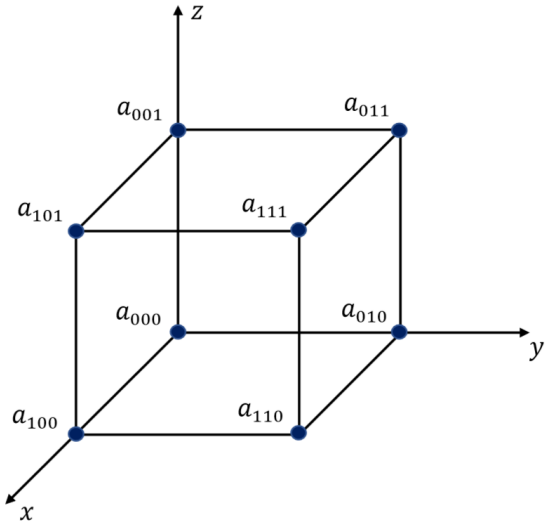

Figure 4.1: Coefficient hypermatrix for a pure state of three qubits.

When moving from matrices to hypermatrices, the place of the determinant is taken by the hyperdeterminant. We will use the second formula for Cayley's hyperdeterminant Det, which is defined as

$$
\begin{aligned}
\mathrm{Det}A = {} & a_{000}^2 a_{111}^2 + a_{001}^2 a_{110}^2 + a_{010}^2 a_{101}^2 + a_{100}^2 a_{011}^2 \\
& - 2a_{000}a_{001}a_{110}a_{111} - 2a_{000}a_{010}a_{101}a_{111} \\
& - 2a_{000}a_{011}a_{100}a_{111} - 2a_{001}a_{010}a_{101}a_{110} \\
& - 2a_{001}a_{011}a_{110}a_{100} - 2a_{010}a_{011}a_{101}a_{100} \\
& + 4a_{000}a_{011}a_{101}a_{110} + 4a_{001}a_{010}a_{100}a_{111}
\end{aligned} \tag{4.4}
$$

As the name suggests, this is not the only formula for the hyperdeterminant that exists, but it is the most commonly used one. Alternatively, we can express Det$A$ using the Levi-Civita symbol ε_{ij} which satisfies $\varepsilon_{01} = -\varepsilon_{10} = 1$ and $\varepsilon_{00} = \varepsilon_{11} = 0$, as follows

$$
\mathrm{Det}A = \frac{1}{2}\sum_{all} a_{i_1i_2i_3}a_{j_1j_2j_3}a_{k_1k_2k_3}a_{l_1l_2l_3}\varepsilon_{i_1j_1}\varepsilon_{i_2j_2}\varepsilon_{k_1l_1}\varepsilon_{k_2l_2}\varepsilon_{i_3k_3}\varepsilon_{j_3l_3} \tag{4.5}
$$

Let us construct a potential entanglement measure based on this quantity.

Definition 4.1. *We define the **3-tangle** of a pure tripartite state* $|\psi\rangle$ *as*

$$
\tau(\psi) = 4|Det\,A| \tag{4.6}
$$

The prefactor 4 ensures the normalization $0 \leq \tau \leq 1$. If the 3-tangle is to be interpreted as a measure of entanglement, it must meet certain prerequisites.

1. A measure of entanglement must vanish for states with no entanglement. Let's consider a product state $|\psi\rangle = |\psi_A\rangle \otimes |\psi_B\rangle \otimes |\psi_C\rangle$. The coefficients of the basis states can be factorized: $a_{i_1 i_2 i_3} = a_{i_1} b_{i_2} c_{i_3}$. Therefore it follows from (4.5) that

$$\mathrm{Det}A \propto \sum_{i_1, j_1} a_{i_1} a_{j_1} \varepsilon_{i_1 j_1} = 0 \tag{4.7}$$

A pure state of two qubits can be either entangled or in a product form. But now the situation is a bit more nuanced, since there is a new middle ground: what if only one of the three qubits can be factored out, leaving the other two in an entangled state? Let's consider for example a state with type A-BC entanglement, i.e. $|\psi\rangle = |\psi_A\rangle \otimes |\psi_{BC}\rangle$. The basis coefficients can be written as $a_{i_1 i_2 i_3} = a_{i_1} b_{i_2 i_3}$ and it is quite simple to verify that we end up with (4.7) again. But how about the converse statement? Can we infer that $|\psi\rangle$ is unentangled if $\tau(\psi) = 0$? The answer is negative, and we will illustrate this later using a straightforward example. However, in light of the interpretation of the 3-tangle, this does not constitute a problem.

2. The 3-tangle has the desirable property of being invariant under permutations of the qubits. It is easy to confirm this property, since these operations amount to merely renaming dummy indices in (4.5).

3. A basic requirement for any measure of entanglement is also the invariance under local unitary transformations (LU's). We will confirm that $|\mathrm{Det}A|$ satisfies that requirement by outlining the proof. If we apply the transformation $U = U_1 \otimes U_2 \otimes U_3 \in \mathrm{SU}(2)^{\otimes 3}$ to the initial $|\psi\rangle$ we get the state

$$\begin{aligned} U|\psi\rangle &= \sum_{i_1 . i_2, i_3} a_{i_1 i_2 i_3} U_1 |i_1\rangle \otimes U_2 |i_2\rangle \otimes U_3 |i_3\rangle \\ &= \sum_{k_1 . k_2, k_3} \left(\sum_{i_1 . i_2, i_3} a_{i_1 i_2 i_3} (U_1)_{i_1 k_1} (U_2)_{i_2 k_2} (U_3)_{i_3 k_3} \right) |k_1 k_2 k_3\rangle \\ &= \sum_{k_1 . k_2, k_3} a'_{k_1 k_2 k_3} |k_1 k_2 k_3\rangle \end{aligned} \tag{4.8}$$

By substituting these primed coefficients in (4.5) we obtain the transformed hyperdeterminant $\mathrm{Det}A'$. Now if we use the unitarity condition

$$\sum_k (U_i)_{\alpha k} (U_i^\dagger)_{k\beta} = \delta_{\alpha\beta} \tag{4.9}$$

as well as the property

$$\varepsilon_{\alpha\beta} \varepsilon_{\gamma\delta} = \delta_{\alpha\gamma} \delta_{\beta\delta} - \delta_{\alpha\delta} \delta_{\beta\gamma} \tag{4.10}$$

we can verify that $|\mathrm{Det}A'|^2 = |\mathrm{Det}A|^2$ thus proving that the modulus of the hyperdeterminant is indeed a local invariant. ■

4. A crucial property for entanglement measures is of course monotonicity, meaning they decrease under local operations and classical communication (LOCC). In order to prove that this holds for the 3-tangle τ, we will follow the outline provided in [18]. Specifically, we will prove that τ is a quantity that decreases on average in the transitions from ψ to ensembles of pure states via local measurements[1]. We consider A_i to be Krauss operators of a local measurement (for example on qubit A) satisfying $A_1 A_1^\dagger + A_2 A_2^\dagger = I$. Then we can write $A_i = U_i D_i V$ for $i = 1, 2$ with U_i and V being unitary, and D_i being diagonal matrices with entries (a, b) and $(\sqrt{1-a^2}, \sqrt{1-b^2})$ respectively. The action of each element A_i on a quantum state $|\psi\rangle$ produces a subnormalized state $|\tilde{\varphi}_i\rangle = A_i |\psi\rangle$. We define the normalized version of this state to be $|\varphi_i\rangle = |\tilde{\varphi}_i\rangle / \sqrt{p_i}$ with $p_i = \langle\tilde{\varphi}_i|\tilde{\varphi}_i\rangle$. Then

$$\langle\tau\rangle = p_1 \tau(\varphi_1) + p_2 \tau(\varphi_2) \tag{4.11}$$

with $\tau(\varphi_i) = \tau(U_i D_i V \psi)$. But as we previously demonstrated, the 3-tangle is invariant under local unitary transformations, so $\tau(U_i D_i V \psi) = \tau(D_i V \psi)$. Let us consider the usual decomposition (4.1) of the initial state $|\psi\rangle$. The transformed state after the application of V has some different coefficients in the computational basis that we denote as $a'_{i_1 i_2 i_3}$. The coefficients of $|\tilde{\varphi}_i\rangle$ are $\tilde{a}''_{i_1 i_2 i_3}$ with

$$\begin{aligned} \tilde{a}''_{0 i_2 i_3} &= (D_i)_{00}\, a'_{0 i_2 i_3} \\ \tilde{a}''_{1 i_2 i_3} &= (D_i)_{11}\, a'_{1 i_2 i_3} \end{aligned} \tag{4.12}$$

And finally, the coefficients of $|\varphi_i\rangle$ are $a''_{i_1 i_2 i_3} = \tilde{a}''_{i_1 i_2 i_3} / \sqrt{p_i}$. Now, because the 3-tangle is quartic in a's, it follows that $\tau(\varphi_i) = \tau(\tilde{\varphi}_i)/p_i^2$. Furthermore, because of $\varepsilon_{i_1 j_1}$ and $\varepsilon_{k_1 l_1}$ in (4.5), we know that every term of τ contains two a's with subscripts starting with 0 and two starting with 1. Combining that with (4.12) we obtain

$$\tau(\varphi_i) = \frac{1}{p_i^2}\tau(\tilde{\varphi}_i) = \frac{(D_i)_{00}^2\,(D_i)_{11}^2}{p_i^2}\tau(V\psi) \tag{4.13}$$

But τ is invariant under local unitaries, so $\tau(V\psi) = \tau(\psi)$. As a consequence

$$\tau(\varphi_i) = \frac{(D_i)_{00}^2\,(D_i)_{11}^2}{p_i^2}\tau(\psi) \tag{4.14}$$

By substituting these values in (4.11) with the proper entries for the diagonal matrices, we obtain

$$\langle\tau\rangle = \left[\frac{a^2 b^2}{p_1} + \frac{\left(1-a^2\right)\left(1-b^2\right)}{p_2}\right]\tau(\psi) \tag{4.15}$$

[1] See Section 1.5

It is

$$\begin{aligned} p_1 &= \langle\tilde{\varphi}_1|\tilde{\varphi}_1\rangle = a^2 P_0 + b^2 P_1 \\ p_2 &= \langle\tilde{\varphi}_2|\tilde{\varphi}_2\rangle = (1-a^2) P_0 + (1-b^2) P_1 \end{aligned} \tag{4.16}$$

with

$$P_0 = \sum_{i_2,i_3} \left|a_{0 i_2 i_3}\right|^2 \quad \text{and} \quad P_1 = \sum_{i_2,i_3} \left|a_{1 i_2 i_3}\right|^2 \tag{4.17}$$

From (4.15) and (4.16), while keeping in mind that $P_0 + P_1 = 1$, it is a matter of algebra to prove $\langle\tau\rangle \leq \tau(\psi)$, thus proving that the 3-tangle is an entanglement monotone. ■

Since the 3-tangle vanishes for product states and the ones with bipartite entanglement, it feels fair to assume that this quantity measures the amount of tripartite entanglement. This assumption is backed up by the value of the 3-tangle for states like the Greenberger-Horne-Zeilinger (GHZ) state

$$|GHZ\rangle = \frac{1}{\sqrt{2}} (|000\rangle + |111\rangle) \tag{4.18}$$

which can be regarded as the maximally entangled state of three qubits, and for which $\tau(GHZ) = 1$. But our interpretation of the 3-tangle as a measure of tripartite entanglement falls apart when we consider states like the W state

$$|W\rangle = \frac{1}{\sqrt{3}} (|001\rangle + |010\rangle + |100\rangle) \tag{4.19}$$

because $\tau(W) = 0$, and clearly none of the three qubits can be factored out. Before we throw our hands in the air, let us investigate further. Perhaps the 3-tangle is able to discern these two states based on a physical property. Suppose we get rid of one qubit from the $|GHZ\rangle$ state, for example qubit C. Then the other two are left in the mixed state

$$\rho_{AB} = \mathrm{Tr}_C \left(|GHZ\rangle \langle GHZ|\right) = \frac{1}{2} \left(|00\rangle \langle 00| + |11\rangle \langle 11|\right) \tag{4.20}$$

We observe that by tracing out one particle, the other two are left in a separable state, i.e. they are not entangled. Equivalently, any measurement of one particle leaves the other two in a product state. The fact that the disposal of an arbitrary particle ruins the entanglement, provides us with insight into the nature of the GHZ state: it possesses what we call *essential 3-way entanglement*, that involves correlations of all three parties simultaneously. We contrast this with what happens when we trace out a particle from the $|W\rangle$ state

$$\rho_{AB} = \mathrm{Tr}_C \left(|W\rangle \langle W|\right) = \frac{1}{3} \left(|\psi^+\rangle \langle \psi^+| + |00\rangle \langle 00|\right) \tag{4.21}$$

where $|\psi^+\rangle$ is the Bell state $|\psi^+\rangle = (|01\rangle + |10\rangle)/\sqrt{2}$. In this case ρ_{AB} is a partially entangled state, meaning that there exists entanglement exclusively between qubits A and B, without any involvement of qubit C. This is called *2-way entanglement*, and it is in fact the only type of entanglement found in the state $|W\rangle$: there is entanglement between qubits A and B, B and C, A and C but not 3-way entanglement involving all three parties. It should be noted that, in general, we meet both kinds of entanglement (2-way and 3-way) in three-qubit states. In the next section, we will deal with the classification of states with tripartite entanglement. We will discover that they belong in one of two equivalence classes: the one with states that possess 3-way entanglement and the one with states that do not. The $|GHZ\rangle$ and $|W\rangle$ states are representatives of their respective class.

At this point one can probably suspect the role of the 3-tangle as a measure of entanglement: it quantifies the amount of essential 3-way entanglement of a given pure state. An indication of that fact is also the invariance of the 3-tangle under permutations of the parties, showing that it does indeed represent a collective property of all three qubits. The exact interpretation of τ will be proven in the next subsection through a very important equation.

There is more to the hypermatrix A than just it's hyperdeterminant. Is there any other information about the entanglement properties that can extracted from the structure of A? The answer is in fact yes. We can identify conditions for all possible factorizations of a quantum state based on characteristics of A. Let us start by rearranging the terms in the quantum state $|\psi\rangle$ to get

$$\begin{aligned}|\psi\rangle &= (a_{000}|00\rangle + a_{010}|01\rangle + a_{100}|10\rangle + a_{110}|11\rangle) \otimes |0\rangle \\ &\quad + (a_{001}|00\rangle + a_{011}|01\rangle + a_{101}|10\rangle + a_{111}|11\rangle) \otimes |1\rangle \\ &= |\psi_{AB}^{(0)}\rangle \otimes |0\rangle + |\psi_{AB}^{(1)}\rangle \otimes |1\rangle \end{aligned} \tag{4.22}$$

with

$$|\psi_{AB}^{(0)}\rangle = \sum_{i_1,i_2} a_{i_1 i_2 0}|i_1 i_2\rangle \quad \text{and} \quad |\psi_{AB}^{(1)}\rangle = \sum_{i_1,i_2} a_{i_1 i_2 1}|i_1 i_2\rangle \tag{4.23}$$

It is obvious that if these two states are linearly dependent, i.e. $|\psi_{AB}^{(1)}\rangle = \lambda|\psi_{AB}^{(0)}\rangle$ for some $\lambda \in \mathbb{C}$, then qubit C can be factored out

$$|\psi\rangle = |\psi_{AB}^{(0)}\rangle \otimes (|0\rangle + \lambda|1\rangle) \tag{4.24}$$

This condition of linear dependence is translated as $a_{i_1 i_2 1} = \lambda a_{i_1 i_2 0}\ \forall\, i_1, i_2$, which is no different than saying $A_{z_1} = \lambda A_{z_0}$. This is to say, if the faces of A lying on the planes $z = 0$ and $z = 1$ are proportionate , then qubit C -which is the one associated with the z axis- can be factored out from the quantum state. This condition is sufficient, but also necessary: if we started with the requirement $|\psi\rangle = |\psi_{AB}\rangle \otimes |\psi_C\rangle$, we would end up with proportionate matrices[2]. We have thus proved the following criterion for bipartite factorization of a pure state:

Theorem 4.2. *In a pure state $|\psi\rangle$ of three qubits, one qubit can be factored out if and only if the sides of the hypermatrix A in the direction associated with this qubit are proportionate.*

[2]proportionality also incorporates the case where one of these two matrices is a zero matrix.

In order to determine an equivalent statement for product states, one simply has to expand the above factorization condition to all three qubits:

Theorem 4.3. *The full factorization of a pure state $|\psi\rangle$ of three qubits is possible if and only if all opposite sides of the hypermatrix A are proportionate.*

Although these criteria are pretty straightforward, it is worth noting that they can be restated in terms of the 3-tangle and the determinants of the sides of A. It can be demonstrated that the proportionality of two opposite sides of A means the determinants of the other four sides, as well as the 3-tangle τ, all vanish (and vise versa). Likewise, full factorization is possible if and only if all the sides of the hypermatrix A have vanishing determinants, and furthermore the 3-tangle is zero. Here the vanishing of pairs of determinants (two and three pairs respectively) is a recurring theme[3]. This begs the question of what effect does the vanishing of a single pair of determinants have on a quantum state, if any at all. To get the answer, let us return to the state $|\psi\rangle$ rearranged as

$$|\psi\rangle = |\psi_{AB}^{(0)}\rangle \otimes |0\rangle + |\psi_{AB}^{(1)}\rangle \otimes |1\rangle \tag{4.25}$$

If next we calculate the reduced density matrix of the subsystem AB, we obtain

$$\rho_{AB} = \mathrm{Tr}_C\left(|\psi\rangle\langle\psi|\right) = |\psi_{AB}^{(0)}\rangle\langle\psi_{AB}^{(0)}| + |\psi_{AB}^{(1)}\rangle\langle\psi_{AB}^{(1)}| \tag{4.26}$$

We turn our attention to these sub-normalized states of the subsystem AB. Suppose that we have a bipartite system in the pure state $|\psi_{AB}^{(0)}\rangle$ (its normalized version to be exact). The coefficient matrix associated with that state is, up to a normalization constant, none other than A_{z_0}, namely, the face of the hypermatrix A lying in the plane $z = 0$. Similarly, the respective matrix for the second state is A_{z_1}. We have already established the fact when the determinant of a 2×2 coefficient matrix is zero, then the corresponding system is in a product state, and vise versa. So,

$$\det A_{z_i} = 0 \implies |\psi_{AB}^{(i)}\rangle = |\psi_A^{(i)}\rangle \otimes |\psi_B^{(i)}\rangle, \quad i = 0, 1 \tag{4.27}$$

If the above is true, then the decomposition of ρ_{AB} in (4.26) becomes one of pure unentangled states, making it separable. In other words, if these two sub-determinants vanish, we lose the 2-way entanglement between particles A and B! Obviously, the concurrence that measures this type of entanglement is zero: $C_{AB} = 0$. However, the converse is not true: the requirement $C_{AB} = 0$ does not necessarily mean that the determinants of A_{z_0} and A_{z_1} are zero. We can use as a counterexample the state

$$|\varphi\rangle = \frac{1}{\sqrt{2}}\left(|\varphi_{AB}^{+}\rangle \otimes |0_C\rangle + |\varphi_{AB}^{-}\rangle \otimes |1_C\rangle\right) = \frac{1}{2}\left(|000\rangle + |110\rangle + |001\rangle - |111\rangle\right) \tag{4.28}$$

with $|\varphi^{\pm}\rangle$ being the Bell states $(|00\rangle \pm |11\rangle)/\sqrt{2}$. By tracing out qubit C we obtain the density matrix

$$\rho_{AB} = \frac{1}{2}\left(|\varphi^{+}\rangle\langle\varphi^{+}| + |\varphi^{-}\rangle\langle\varphi^{-}|\right) = \frac{1}{2}\left(|00\rangle\langle 00| + |11\rangle\langle 11|\right) \tag{4.29}$$

[3] we refer to a pair of determinants when speaking about the determinants of opposite sides of A

which is clearly unentangled, with $C_{AB} = 0$. It is quite easy to calculate that for this state $\det A_{z_0} = 1/4$ and $\det A_{z_1} = -1/4$, so both do not vanish. In conclusion, the vanishing of a pair of determinants is a sufficient, but stronger than necessary condition for the absence of a certain type of 2-way entanglement.

$$\begin{aligned} \det A_{z_0} = \det A_{z_1} = 0 &\implies C_{AB} = 0 \\ \det A_{y_0} = \det A_{y_1} = 0 &\implies C_{AC} = 0 \\ \det A_{x_0} = \det A_{x_1} = 0 &\implies C_{BC} = 0 \end{aligned} \tag{4.30}$$

4.2 Distribution of Entanglement and a Triangle Measure

In this subsection we will calculate all the reduced density matrices that result from tracing out one or two qubits from the general pure three-qubit state. The results will help us obtain analytic expressions for all the relevant concurrences. Most importantly, an equation will arise that establishes the role of the three-tangle as a measure of essential 3-way entanglement. Let's consider the case where we trace out qubit C. That operation leaves us with the following density matrix ρ_{AB} which describes the subsystem AB

$$\begin{aligned} \rho_{AB} &= \mathrm{Tr}_C \, |\psi\rangle \langle\psi| \\ &= \mathrm{Tr}_C \sum_{i_1,i_2,i_3} \sum_{j_1,j_2,j_3} a_{i_1 i_2 i_3} a^*_{j_1 j_2 j_3} \, |i_1 i_2 i_3\rangle \langle j_1 j_2 j_3| \\ &= \sum_{k_3} \sum_{i_1,i_2} \sum_{j_1,j_2} a_{i_1 i_2 k_3} a^*_{j_1 j_2 k_3} \, |i_1 i_2\rangle \langle j_1 j_2| \end{aligned} \tag{4.31}$$

The elements of ρ_{AB} are therefore

$$(\rho_{AB})_{i_1 i_2, j_1 j_2} = \sum_{k_3} a_{i_1 i_2 k_3} a^*_{j_1 j_2 k_3} \tag{4.32}$$

Instead of referring to a line/column of the matrix with two subscripts, we can use the lexicographic order to replace i_1, i_2 with a single subscript i taking values in the range $\{0, 1, 2, 3\}$. We write

$$(\rho_{AB})_{ij} = \sum_{k_3} a_{ik_3} a^*_{jk_3} = \sum_{k_3} (A_{AB-C})_{ik_3} \left(A^\dagger_{AB-C}\right)_{k_3 j} \tag{4.33}$$

If it was not clear before, it surely is now that a matrix product has emerged

$$\rho_{AB} = A_{AB-C} A^\dagger_{AB-C} \tag{4.34}$$

where A_{AB-C} is the matrix

$$A_{AB-C} = \begin{pmatrix} a_{000} & a_{001} \\ a_{010} & a_{011} \\ a_{100} & a_{101} \\ a_{110} & a_{111} \end{pmatrix} \tag{4.35}$$

This of course is not surprising, because we can choose to view $|\psi\rangle$ as a state describing a bipartite system that consists of the 4-level subsystem AB and qubit C. Then A_{AB-C} is simply the 4×2 coefficient matrix of that bipartite state, and (4.34) is to be expected. By repeating these calculations for the other party we find

$$\rho_C = A^T_{AB-C} A^*_{AB-C} \tag{4.36}$$

Similarly, for the other partitions of the system ABC we have

$$\begin{aligned} \rho_{AC} &= A_{AC-B} A^\dagger_{AC-B}\,, \quad & \rho_B &= A^T_{AC-B} A^*_{AC-B} \\ \rho_{BC} &= A_{BC-A} A^\dagger_{BC-A}\,, \quad & \rho_A &= A^T_{BC-A} A^*_{BC-A} \end{aligned} \tag{4.37}$$

with the respective coefficient matrices

$$A_{AC-B} = \begin{pmatrix} a_{000} & a_{010} \\ a_{001} & a_{011} \\ a_{100} & a_{110} \\ a_{101} & a_{111} \end{pmatrix}, \quad A_{BC-A} = \begin{pmatrix} a_{000} & a_{100} \\ a_{001} & a_{101} \\ a_{010} & a_{110} \\ a_{011} & a_{111} \end{pmatrix} \tag{4.38}$$

Obviously qubit C can be entangled with the system AB. But how can we quantify this type of entanglement? Thus far we have only defined concurrence for a pair of qubits, but now one part of the bipartite system has a four-dimensional state space. However, due to C being a single qubit, ρ_{AB} does not utilize the full space: it has at most two non-zero eigenvalues, or equivalently $r(\rho_{AB}) \leq 2$. So, in this context, we might as well think of AB as a "second qubit", hence concurrence is well defined. Since the full system is in a pure state, we have

$$C^2_{AB-C} = 4 \det \rho_C = 2\left(1 - \operatorname{Tr} \rho_C^2\right) = 4 \sum \tau_{AB-C} \tag{4.39}$$

In the last step we expressed the concurrence in terms of the coefficients of $|\psi\rangle$, with τ_{AB-C} being the 2-tangles resulting from the six minors of A_{AB-C}.

If we want to quantify the entanglement between qubits A and B exclusively, we have to use the formula for the concurrence of mixed states

$$C_{AB} = \max\{0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}\} \tag{4.40}$$

where λ_i are the eigenvalues of $\rho_{AB}\tilde{\rho}_{AB}$ in decreasing order. But as we discussed, there are only two non-zero eigenvalues of ρ_{AB}, and as a consequence the same is true for $\rho_{AB}\tilde{\rho}_{AB}$. Thus, for an entangled mixed state of AB

$$\begin{aligned} C_{AB} &= \sqrt{\lambda_1} - \sqrt{\lambda_2} \\ \implies C^2_{AB} &= \lambda_1 + \lambda_2 - 2\sqrt{\lambda_1 \lambda_2} = \operatorname{Tr}(\rho_{AB}\tilde{\rho}_{AB}) - 2\sqrt{\lambda_1 \lambda_2} \end{aligned} \tag{4.41}$$

Let us concentrate on the trace for a moment. The spin-flipped matrix $\tilde{\rho}_{AB}$ is defined as

$$\tilde{\rho}_{AB} = \left(\sigma_y \otimes \sigma_y\right) \rho^*_{AB} \left(\sigma_y \otimes \sigma_y\right) \tag{4.42}$$

The tensor product of the Pauli matrix σ_y with itself is a matrix acting on the tensor product of the individual Hilbert spaces

$$\sigma_y \otimes \sigma_y = \sum_{i_1,i_2} \sum_{j_1,j_2} \left(\sigma_y \otimes \sigma_y\right)_{i_1 i_2, j_1 j_2} |i_1 i_2\rangle \langle j_1 j_2| \tag{4.43}$$

with elements

$$\left(\sigma_y \otimes \sigma_y\right)_{i_1 i_2, j_1 j_2} = (\sigma_y)_{i_1, j_1} (\sigma_y)_{i_2, j_2} = (-i\varepsilon_{i_1 j_1})(-i\varepsilon_{i_2 j_2}) = -\varepsilon_{i_1 j_1}\varepsilon_{i_2 j_2} \tag{4.44}$$

Now with the help of (4.34) and (4.44) we can compute the elements of $\rho_{AB}\tilde{\rho}_{AB}$

$$\begin{aligned}(\rho_{AB}\tilde{\rho}_{AB})_{i_1 i_2, j_1 j_2} &= \sum (\rho_{AB})_{i_1 i_2, k_1 k_2} \left(\sigma_y \otimes \sigma_y\right)_{k_1 k_2, l_1 l_2} (\rho^*_{AB})_{l_1 l_2, m_1 m_2} \left(\sigma_y \otimes \sigma_y\right)_{m_1 m_2, j_1 j_2} \\ &= \sum a_{i_1 i_2 i_3} a^*_{k_1 k_2 i_3} \varepsilon_{k_1 l_1} \varepsilon_{k_2 l_2} a^*_{l_1 l_2 j_3} a_{m_1 m_2 j_3} \varepsilon_{m_1 j_1} \varepsilon_{m_2 j_2}\end{aligned} \tag{4.45}$$

where we sum over all repeated indices. We move on to calculating the trace

$$\begin{aligned}\mathrm{Tr}(\rho_{AB}\tilde{\rho}_{AB}) &= \sum_{i_1,i_2} (\rho_{AB}\tilde{\rho}_{AB})_{i_1 i_2, i_1 i_2} \\ &= \sum_{\text{all}} a_{i_1 i_2 i_3} a^*_{k_1 k_2 i_3} \varepsilon_{k_1 l_1} \varepsilon_{k_2 l_2} a^*_{l_1 l_2 j_3} a_{m_1 m_2 j_3} \varepsilon_{m_1 i_1} \varepsilon_{m_2 i_2}\end{aligned} \tag{4.46}$$

And by performing the substitutions

$$\begin{aligned}\varepsilon_{k_1 l_1} \varepsilon_{m_1 i_1} &= \delta_{k_1 m_1} \delta_{l_1 i_1} - \delta_{k_1 i_1} \delta_{l_1 m_1} \\ \varepsilon_{k_2 l_2} \varepsilon_{m_2 i_2} &= \delta_{k_2 m_2} \delta_{l_2 i_2} - \delta_{k_2 i_2} \delta_{l_2 m_2}\end{aligned} \tag{4.47}$$

we have

$$\begin{aligned}\mathrm{Tr}(\rho_{AB}\tilde{\rho}_{AB}) &= \sum_{\text{all}} a_{i_1 i_2 i_3} a^*_{k_1 k_2 i_3} a^*_{l_1 l_2 j_3} a_{m_1 m_2 j_3} \left(\delta_{k_1 m_1} \delta_{l_1 i_1} - \delta_{k_1 i_1} \delta_{l_1 m_1}\right) \left(\delta_{k_2 m_2} \delta_{l_2 i_2} - \delta_{k_2 i_2} \delta_{l_2 m_2}\right) \\ &= \sum_{\text{all}} a_{i_1 i_2 i_3} a^*_{k_1 k_2 i_3} a^*_{i_1 i_2 j_3} a_{k_1 k_2 j_3} - \sum_{\text{all}} a_{i_1 i_2 i_3} a^*_{k_1 i_2 i_3} a^*_{i_1 l_2 j_3} a_{k_1 l_2 j_3} \\ &\quad - \sum_{\text{all}} a_{i_1 i_2 i_3} a^*_{i_1 k_2 i_3} a^*_{l_1 i_2 j_3} a_{l_1 k_2 j_3} + \sum_{\text{all}} a_{i_1 i_2 i_3} a^*_{i_1 i_2 i_3} a^*_{l_1 l_2 j_3} a_{l_1 l_2 j_3} \\ &= \mathrm{Tr}\,\rho_C^2 - \mathrm{Tr}\,\rho_A^2 - \mathrm{Tr}\,\rho_B^2 + 1 \\ &= 1 - \mathrm{Tr}\,\rho_A^2 + 1 - \mathrm{Tr}\,\rho_B^2 - \left(1 - \mathrm{Tr}\,\rho_C^2\right) \\ &= \frac{1}{2}\left(C^2_{BC-A} + C^2_{AC-B} - C^2_{AB-C}\right)\end{aligned} \tag{4.48}$$

Having copmuted the above trace, we are left with the task of figuring out an expression for the quantity $\lambda_1\lambda_2$, which is the product of the non-zero eigenvalues of the matrix $\rho_{AB}\tilde{\rho}_{AB}$. If these were the only eigenvalues, we would simply be speaking about its determinant, but that

is not the case. However, this problem can be overcome if we restrict the action of the matrix to its range. In this subspace, $\rho_{AB}\tilde{\rho}_{AB}$ is represented by a 2×2 matrix R, and $\lambda_1\lambda_2$ is indeed the determinant of R. The range of $\rho_{AB}\tilde{\rho}_{AB}$ (which is the same as the range of ρ_{AB}) is spanned by the two vectors

$$|u_0\rangle = |\psi^{(0)}_{AB}\rangle = \sum_{i_1,i_2} a_{i_1 i_2 0}\,|i_1 i_2\rangle \quad \text{and} \quad |u_1\rangle = |\psi^{(1)}_{AB}\rangle = \sum_{i_1,i_2} a_{i_1 i_2 1}\,|i_1 i_2\rangle \tag{4.49}$$

The elements of R are thus given by

$$R_{ij} = \langle u_i|\rho_{AB}\tilde{\rho}_{AB}|u_j\rangle = \sum a_{k_1 k_2 j}\, a^*_{l_1 l_2 i}\, a^*_{m_1 m_2 k_3}\, a_{n_1 n_2 k_3}\, \varepsilon_{l_1 m_1}\, \varepsilon_{l_2 m_2}\, \varepsilon_{n_1 k_1}\, \varepsilon_{n_2 k_2} \tag{4.50}$$

Now we are in a position to calculate the determinant of R, arriving at a very interesting result

$$\sqrt{\lambda_1\lambda_2} = \sqrt{\det R} = \frac{\tau}{4} \tag{4.51}$$

Combining (4.41), (4.48) and (4.51) we finally attain a formula for the concurrence of the bipartite subsystem AB

$$C^2_{AB} = \frac{1}{2}\left(C^2_{BC-A} + C^2_{AC-B} - C^2_{AB-C} - \tau\right) \tag{4.52}$$

One can repeat these calculations for the other 2-qubit subsystems, or simply argue that by symmetry we must have

$$C^2_{AC} = \frac{1}{2}\left(C^2_{BC-A} + C^2_{AB-C} - C^2_{AC-B} - \tau\right) \tag{4.53}$$

$$C^2_{BC} = \frac{1}{2}\left(C^2_{AB-C} + C^2_{AC-B} - C^2_{BC-A} - \tau\right) \tag{4.54}$$

The relations (4.52)-(4.54) are of the utmost significance, because they explain how entanglement is being distributed between the three parties of the system ABC. But perhaps this physical interpretation becomes more clear if we blend them together to obtain

$$C^2_{AB-C} = C^2_{AC} + C^2_{BC} + \tau \tag{4.55}$$

as well as its symmetric counterparts. The interpretation is quite simple and elegant: the entanglement between C and AB is the sum of the entanglement of C with A and B separately, plus an amount of entanglement that cannot be accounted for by correlations of any pairs of qubits. The quantity that measures this type of essential 3-way entanglement is none other that the 3-tangle, which is also referred to as *residual tangle*. From (4.55) it is clear that the following inequality holds

$$C^2_{AC} + C^2_{BC} \leq C^2_{AB-C} \tag{4.56}$$

This describes what we term the *monogamy* of entanglement. Quantum correlations cannot be freely shared between the three parties of the system. If, for example, qubits A and C are

maximally entangled, then that leaves no room for any entanglement between them and qubit B whatsoever. The existence of some type of entanglement constraints all the other types to some degree.

Concurrence Triangle and a Measure for Tripartite Entanglement

From the relations (4.52)-(4.54) we obtain the inequalities

$$C^2_{ij-k} \leq C^2_{ik-j} + C^2_{jk-i} \tag{4.57}$$

where i, j, k can represent A, B, C or any other permutation of the three qubits. The above inequality has a simple geometric interpretation: these squared concurrences can be considered as the sides of a triangle, known as the *concurrence triangle*.

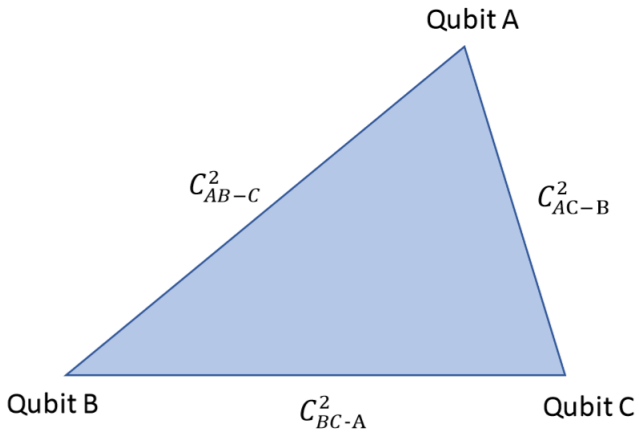

Figure 4.2: The concurrence triangle

This prompts the question: can geometric properties of this triangle be used to quantify tripartite entanglement? Initially, we explore the perimeter P of the triangle, referred to as the *global entanglement*, given by:

$$P = C^2_{AB-C} + C^2_{BC-A} + C^2_{AC-B} = 2\left(C^2_{AB} + C^2_{AC} + C^2_{BC}\right) + 3\tau \tag{4.58}$$

However, it fails as an entanglement measure since biseparable states, devoid of tripartite entanglement, yield non-zero perimeters. For instance

$$|\psi_{ABC}\rangle = |\psi_A\rangle \otimes |\psi_{BC}\rangle \implies P = 2C^2_{BC} \neq 0 \tag{4.59}$$

On the contrary, in a recent article [20] the *area* of the concurrence triangle was proposed as a viable measure of tripartite entanglement. It was demonstrated that the area is zero if and only if at least one of its edges has zero length, implying qubit factorization from the state. Consequently, we introduce the following theorem:

Theorem 4.4. *The square root of the area of the concurrence triangle is a genuine tripartite entanglement measure. Employing Heron's formula for triangle area, we define the concurrence fill as*

$$F_{ABC} = \left[\frac{16}{3} Q\left(Q - C^2_{AB-C}\right)\left(Q - C^2_{AC-B}\right)\left(Q - C^2_{BC-A}\right)\right]^{1/4} \tag{4.60}$$

where Q represents the half-perimeter of the triangle

This measure ranges between 0 and 1, vanishing if and only if the state is unentangled. Furthermore, the exponent of 1/4 ensures monotonicity under LOCC, fulfilling all criteria for entanglement measures. It also possesses another desirable property: it ranks the GHZ state as the maximally entangled state for three qubits. This state is more effective than W at faithfully teleporting an arbitrary single-qubit state.

As expected, for states like the GHZ, that only contain 3-way entanglement, the above triangle measure reduces to the 3-tangle. If, for example, we consider the generalized GHZ state

$$|GHZ(p)\rangle = \sqrt{p}\,|000\rangle + \sqrt{1-p}\,|111\rangle \tag{4.61}$$

then

$$F_{ABC} = \tau = 4p\,(1-p) \tag{4.62}$$

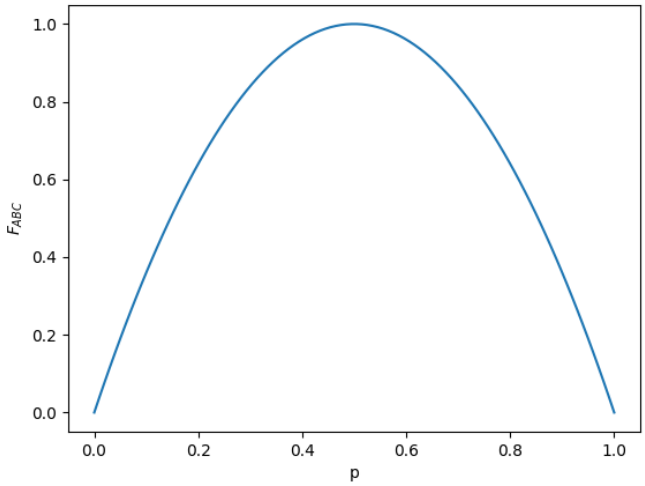

Figure 4.3: Values of the concurrence fill for the single parameter p in the generalized GHZ state

4.3 SLOCC Classification

In [18] a framework was introduced that can be used to classify pure states of multipartite systems in different entanglement classes. These are called equivalence classes, and states in the same class exhibit similar entanglement properties. Two states in the same class are equivalent in the sense that we can convert from one to the other through local operations and classical communication (LOCC) with non-vanishing probability. This is referred to as stochastic equivalence, and the operations as SLOCC (stochastic LOCC). However, states that belong in a different class cannot be converted into each other by means of LOCC, not even

with very small probability of success.

It was shown that two states $|\varphi\rangle$ and $|\psi\rangle$ are equivalent under SLOCC if and only if there exists an invertible local operator (ILO) relating them. For tripartite systems this relation would look like

$$|\varphi\rangle = A \otimes B \otimes C\,|\psi\rangle \tag{4.63}$$

where each of the operators A, B and C is applied locally by each party, and is invertible:

$$|\psi\rangle = A^{-1} \otimes B^{-1} \otimes C^{-1}\,|\varphi\rangle \tag{4.64}$$

A main mathematical tool in this study will be the ranks of the reduced density matrices $r(\rho_A), r(\rho_B)$ and $r(\rho_C)$. The reason is that these local ranks are invariant under ILO. Therefore, states with different local ranks are inequivalent under SLOCC, since they cannot possibly be related through ILO. For qubits, there are only two possibilities for the rank of the reduced density matrix: i) $r(\rho_k) = 1$ meaning the qubit k is in a pure state and can be factored out of the total state $|\psi\rangle$, and i)) $r(\rho_k) = 2$ indicating the existence of entanglement involving this qubit. Next we present a summary of the main results of the original paper. Pure states of three qubits belong in one of six inequivalent entanglement classes:

- **Class A-B-C (product states)** This class includes completely factorized states, where all the local ranks are equal to 1: $r(\rho_A) = r(\rho_B) = r(\rho_C) = 1$. All these states can be taken, using a particular LU operation, into the form

$$|\psi_{A-B-C}\rangle = |000\rangle \tag{4.65}$$

- **Classes A-BC, AB,C and C-AB (bipartite entanglement)** These are states that contain only bipartite entanglement, and as a result, one of the qubits can be factored out. This qubit corresponds to a reduced density matrix of rank 1, while the other two have full ranks of 2. If we suppose that Alice is the one in possession of the unentangled qubit, then LU operations allow us to uniquely express states of the class A-BC as

$$|\psi_{A-BC}\rangle = |0\rangle \otimes (c_\delta\,|00\rangle + s_\delta\,|11\rangle) \tag{4.66}$$

with $c_\delta \geq s_\delta > 0$. We choose the maximally entangled state

$$\frac{1}{\sqrt{2}}\,|0\rangle \otimes (|00\rangle + |11\rangle) \tag{4.67}$$

as the representative of the class A-BC. All the other states within this class can be obtained from this state with certainty by means of LOCC.

Finally, there is the more interesting case of tripartite entanglement, where all the reduced density matrices have full ranks. But can we say that all states with tripartite entanglement constitute an equivalence class? We already know that this is not true, because there is a meaningful distinction to be made: there are states like the GHZ state with genuine 3-way entanglement, and states like W with only 2-way entanglement. However, local ranks are insufficient to make that distinction, meaning we need a different tool. We can observe that the GHZ and W states have different numbers of product terms in (4.18) and (4.19), namely 2 and 3 product terms respectively. It turns out that equivalence classes can be determined from the minimal number of terms in the product decomposition of a state, because this quantity remains unchanged under SLOCC. With that being said, the set of all states with tripartite entanglement can be separated into two insequivalent classes

1. **GHZ class**: These states have product state decompositions containing at minimum two product vectors. The GHZ state is a representative of the class, hence the name. Any state $|\psi\rangle$ in this class can be taken with LU into a standard product form

$$|\psi_{GHZ}\rangle = \sqrt{K}\left(c_\delta |000\rangle + s_\delta e^{i\varphi} |\varphi_A\rangle |\varphi_B\rangle |\varphi_C\rangle\right) \tag{4.68}$$

where

$$\begin{aligned} |\varphi_A\rangle &= c_\alpha |0\rangle + s_\alpha |1\rangle \\ |\varphi_B\rangle &= c_\beta |0\rangle + s_\beta |1\rangle \\ |\varphi_C\rangle &= c_\gamma |0\rangle + s_\gamma |1\rangle \end{aligned} \tag{4.69}$$

Here K is a normalization factor which is equal to $K = \left(1 + 2c_\delta s_\delta c_\alpha c_\beta c_\gamma c_\varphi\right)^{-1} \in (1/2, \infty)$. The five parameters take values in the ranges $\delta \in (0, \pi/4]$, $\alpha, \beta, \gamma \in (0, \pi/2]$ and $\varphi \in [0, 2\pi)$. Any state that can be expressed in this form belongs in the same equivalence class under SLOCC as GHZ. We can verify that the ILO

$$Q_{GHZ} = \sqrt{2K}\begin{pmatrix} c_\delta & s_\delta c_\alpha e^{i\varphi} \\ 0 & s_\delta s_\alpha e^{i\varphi} \end{pmatrix} \otimes \begin{pmatrix} 1 & c_\beta \\ 0 & s_\beta \end{pmatrix} \otimes \begin{pmatrix} 1 & c_\gamma \\ 0 & s_\gamma \end{pmatrix} \tag{4.70}$$

when applied to $|GHZ\rangle$ indeed produces $|\psi_{GHZ}\rangle$.

$$\begin{aligned} Q_{GHZ}|GHZ\rangle &= \sqrt{2K}\begin{pmatrix} c_\delta & s_\delta c_\alpha e^{i\varphi} \\ 0 & s_\delta s_\alpha e^{i\varphi} \end{pmatrix} \otimes \begin{pmatrix} 1 & c_\beta \\ 0 & s_\beta \end{pmatrix} \otimes \begin{pmatrix} 1 & c_\gamma \\ 0 & s_\gamma \end{pmatrix} \frac{1}{\sqrt{2}} \left(|000\rangle + |111\rangle\right) \\ &= \sqrt{K}\left\{c_\delta |000\rangle + s_\delta e^{i\varphi} \left(c_\alpha |0\rangle + s_\alpha |1\rangle\right) \otimes \left(c_\beta |0\rangle + s_\beta |1\rangle\right) \otimes \left(c_\gamma |0\rangle + s_\gamma |1\rangle\right)\right\} \\ &= \sqrt{K}\left\{c_\delta |000\rangle + s_\delta e^{i\varphi} |\varphi_A\rangle \otimes |\varphi_B\rangle \otimes |\varphi_C\rangle\right\} \\ &= |\psi_{GHZ}\rangle \end{aligned} \tag{4.71}$$

2. **W class**: States in this class cannot be expressed in a decomposition of product states containing only two terms. We choose as a representative of this class the state W.Any state in this class can be taken through LU into the standard form

$$|\psi_W\rangle = \sqrt{a}\,|001\rangle + \sqrt{b}\,|010\rangle + \sqrt{c}\,|100\rangle + \sqrt{d}\,|000\rangle \tag{4.72}$$

with $a, b, c > 0$ and $d = 1 - (a + b + c) \geq 0$. This standard form can be obtained by applying the following ILO to the $|W\rangle$ state

$$Q_W = \begin{pmatrix} \sqrt{a} & \sqrt{d} \\ 0 & \sqrt{c} \end{pmatrix} \otimes \begin{pmatrix} \sqrt{3} & 0 \\ 0 & \frac{\sqrt{3b}}{\sqrt{a}} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{4.73}$$

$$\begin{aligned} Q_W\,|W\rangle &= \begin{pmatrix} \sqrt{a} & \sqrt{d} \\ 0 & \sqrt{c} \end{pmatrix} \otimes \begin{pmatrix} \sqrt{3} & 0 \\ 0 & \frac{\sqrt{3b}}{\sqrt{a}} \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \frac{1}{\sqrt{3}} \left(|001\rangle + |010\rangle + |100\rangle\right) \\ &= \frac{1}{\sqrt{3}} \left\{ \sqrt{a}\,|0\rangle \otimes \sqrt{3}\,|0\rangle \otimes |1\rangle + \sqrt{a}\,|0\rangle \otimes \frac{\sqrt{3b}}{\sqrt{a}}\,|1\rangle \otimes |0\rangle + \left(\sqrt{d}\,|0\rangle + \sqrt{c}\,|1\rangle\right) \otimes \sqrt{3}\,|0\rangle \otimes |0\rangle \right\} \\ &= \sqrt{a}\,|001\rangle + \sqrt{b}\,|010\rangle + \sqrt{c}\,|100\rangle + \sqrt{d}\,|000\rangle \\ &= |\psi_W\rangle \end{aligned} \tag{4.74}$$

There is another way to look at SLOCC classification that is more closely related to our subject of interest. We have established that any difference in the local ranks of two states implies inequivalence under SLOCC. Let us compare for example states from the A-BC and AB-C classes. Any state $|\psi_{A-BC}\rangle$ in the first class has $r(\rho_A) = 1$ which implies vanishing von Neumann entropy: $S(\rho_A) = 0$. For any state $|\psi_{AB-C}\rangle$ in the second class, the respective von Neumann entropy has some positive value $S(\rho_A) > 0$. If these two states were equivalent, we should be able to obtain $|\psi_{AB-C}\rangle$ from $|\psi_{A-BC}\rangle$ through LOCC with some finite probability. But that transformation would take us from a state with $S(\rho_A) = 0$ to one with $S(\rho_A) > 0$. We know this is impossible, since the von Neumann entropy is an entanglement monotone, i.e. it does not increase under LOCC. We conclude that values of entanglement measures can be used to identify equivalence classes. Is there an entanglement measure that can distinguish between the two classes with tripartite entanglement? As we have hinted already, the answer is yes, and it is none other than the 3-tangle. We can do the calculation and confirm that for a state in the GHZ class expressed in the standard product form (4.68) the 3-tangle takes the value

$$\tau(\psi_{GHZ}) = \left(2K s_\alpha s_\beta s_\gamma s_\delta c_\delta\right)^2 \neq 0 \tag{4.75}$$

while it vanishes for any state in the W class. Knowing the role of the 3-tangle, it follows that the GHZ class contains all the states with essential 3-way entanglement, while the rest belong in the W class.

We know that local ranks are invariant under ILO's. But what happens when non-invertible operations are applied? An increase in any local rank would imply an increase in the respective von Neumann entropy, thereby violating monotonicity. Consequently, local ranks can only diminish under such operations. Specifically, when a non-invertible operator acts on a state belonging to the GHZ or W class, it inevitably reduces at least one of the local ranks. The resultant state either has bipartite entanglement, aligning with one of the previously mentioned

classes, or completely loses its entanglement. Similarly, non-invertible local operations have the capability to transform states with bipartite entanglement into product states.

In summary, the set of pure three-qubit states can be divided through SLOCC into 6 inequivalent classes, that form a three-level hierarchical structure as shown in Figure 4.2. At the top of the hierarchy we find two inequivalent classes of tripartite entanglement, namely the GHZ and W classes. The second level contains the three classes of states with bipartite entanglement. These states can be accessed from states in the GHZ and W classes through non-invertible operations. At the bottom of the hierarchy we find product states with no entanglement at all. In order to determine the entanglement class of a state $|\psi\rangle$ all we have to do is follow a simple recipe:

i) Check whether the von Neumann entropy vanishes for any of the three qubits. For that purpose it is sufficient to just check the determinants of the reduced density matrices. If $\det \rho_k = 0$, then qubit k can be separated from the overall wavefunction.

ii) If none of these determinants vanish, then the state has tripartite entanglement. We next compute the 3-tangle: if $\tau(\psi) \neq 0$ then the state falls in the GHZ class (exhibits 3-way entanglement), otherwise it belongs in the W class.

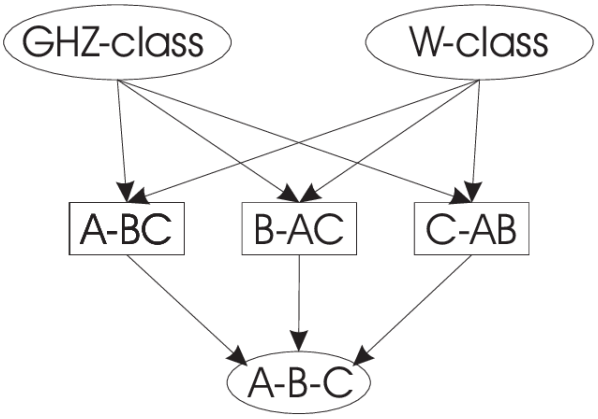

Figure 4.4: The hierarchy of pure states of three qubits. The arrows indicate possible ways to diminish entanglement by means of non-invertible local operations.

4.4 Strong Subadditivity of the von Neumann Entropy

Subadditivity

The Shannon entropy of two random variables X, Y is subadditive, meaning

$$H(X,Y) \leq H(X) + H(Y) \tag{4.76}$$

We will prove that the property of subadditivity also holds for the von Neumann entropy of bipartite systems:

$$S(\rho_{AB}) \leq S(\rho_A) + S(\rho_B) \tag{4.77}$$

This, of course, is not a surprise. The above relation simply tells us that the composite system is more orderly, and contains more information than the individual parts. We will prove it by utilizing the concept of the relative entropy. Let us evaluate the relative entropy between an arbitrary bipartite state ρ_{AB} and the product state $\rho_A \otimes \rho_B$, using the identity

$$\log(\rho_A \otimes \rho_B) = \log \rho_A \otimes I_B + \log \rho_B \otimes I_A \tag{4.78}$$

By the definition (3.16) we have

$$\begin{aligned} S(\rho_{AB} \| \rho_A \otimes \rho_B) &= \mathrm{Tr}\, \rho_{AB} \log \rho_{AB} - \mathrm{Tr}\left\{\rho_{AB} (\log \rho_A \otimes I_B + \log \rho_B \otimes I_A)\right\} \\ &= -S(\rho_{AB}) - \mathrm{Tr}_A (\rho_A \log \rho_A) - \mathrm{Tr}_B (\rho_B \log \rho_B) \\ &= -S(\rho_{AB}) + S(\rho_A) + S(\rho_B) \end{aligned} \tag{4.79}$$

From the positivity of relative entropy follows the desired result ■.

Triangle Inequality

Subadditivity can be used to demonstrate another important property of the von Neumann entropy, namely, that it satisfies the *triangle inequality*

$$S(\rho_{AB}) \geq |S(\rho_A) - S(\rho_B)| \tag{4.80}$$

This is a property unique to the quantum world. There is no classical equivalent, as it does not hold for the Shannon entropy. To prove (4.80) we will first take advantage of the purification theorem. We imagine that the system AB in the state ρ_{AB} (pure or mixed) is part of a larger system ABC in a pure state. One can always choose to view the large system as a bipartite one, consisting, for example, of subsystems A and BC. We know from the Schmidt decomposition that complementary subsystems have equal entropies: $S(\rho_{BC}) = S(\rho_A)$. Obviously the same can be said for the other two bipartite partitions of ABC. From the subadditivity it follows

$$S(\rho_{BC}) = S(\rho_A) \leq S(\rho_B) + S(\rho_C) = S(\rho_B) + S(\rho_{AB}) \implies S(\rho_{AB}) \geq S(\rho_A) - S(\rho_B) \tag{4.81}$$

With the same arguments for the system B-AC we arrive at $S(\rho_{AB}) \geq S(\rho_B) - S(\rho_A)$. Combining these two inequalities for $S(\rho_{AB})$ we arrive at $S(\rho_{AB}) \geq |S(\rho_A) - S(\rho_B)|$ ■.

Strong Subadditivity of von Neumann Entropy

By partitioning a composite system into more than two subsystems we find new inequalities. It has been shown by Lieb [21] that for tripartite systems, the von Neumann entropy satisfies a stronger subbaditivity than (4.77), which is

$$S(\rho_{ABC}) \leq S(\rho_{AB}) + S(\rho_{BC}) \tag{4.82}$$

In order to prove this statement, we will employ two theorems from linear algebra, which we state, but do not prove.

Theorem 4.5. *(Klein's inequality) For positive operators A,B*

$$\mathrm{Tr}\, A\,(\log A - \log B) \geq \mathrm{Tr}\,(A - B) \tag{4.83}$$

with equality if and only if A = B.

Theorem 4.6. *(Golden-Thompson-Syzmanzik) For self-adjoint matrices A and B*

$$\mathrm{Tr}\left(e^A e^B\right) \geq \mathrm{Tr}\left(e^{A+B}\right) \tag{4.84}$$

with equality holding if and only if A and B commute.

We apply Klein's inequality for the particular choice $A = \rho_{ABC}$ and $B = \exp(\log\rho_{AB} + \log\rho_{BC})$. Both operators act on the joint Hilbert space $\mathcal{H}_{ABC}$, but in the last case we omit to write the missing identity operators for the sake of simplicity (for example, we simply write $\log\rho_{AB}$ instead of $\log\rho_{AB}\otimes I_C$). The left-hand side of the inequality becomes

$$\begin{aligned}\mathrm{Tr}\, A\,(\log A - \log B) &= \mathrm{Tr}\,\{\rho_{ABC}\,(\log\rho_{ABC} - \log\rho_{AB} - \log\rho_{BC})\}\\ &= \mathrm{Tr}\,\rho_{ABC}\log\rho_{ABC} - \mathrm{Tr}_{AB}\,\rho_{AB}\log\rho_{AB} - \mathrm{Tr}_{BC}\,\rho_{BC}\log\rho_{BC}\\ &= -S(\rho_{ABC}) + S(\rho_{AB}) + S(\rho_{BC})\end{aligned} \tag{4.85}$$

Then from (4.83) and (4.84) we obtain

$$\begin{aligned}-S(\rho_{ABC}) + S(\rho_{AB}) + S(\rho_{BC}) &\geq \mathrm{Tr}\,\{\rho_{ABC} - \exp(\log\rho_{AB} + \log\rho_{BC})\}\\ &= 1 - \mathrm{Tr}\exp(\log\rho_{AB} + \log\rho_{BC})\\ &\geq 1 - \mathrm{Tr}\,(\rho_{AB}\rho_{BC})\\ &= 1 - \mathrm{Tr}_B\,\rho_B^2 = 0 \quad \blacksquare\end{aligned} \tag{4.86}$$

The inequality (4.82) can be improved.

Theorem 4.7. *(Lieb's Triple Matrix Inequality) For positive matrices R, S, T*

$$\mathrm{Tr}\exp(\log R - \log S + \log T) \leq \mathrm{Tr}\int_0^\infty R\,\frac{1}{S+uI}\,T\,\frac{1}{S+uI}\,du \tag{4.87}$$

Theorem 4.8. *(Strong Subadditivity)*

$$S(\rho_{ABC}) + S(\rho_B) \leq S(\rho_{AB}) + S(\rho_{BC}) \tag{4.88}$$

Proof The proof follows a similar pattern with the previous one, only we make use of Theorem 4.6 this time. We start by applying Klein's inequality for the operators $A = \rho_{ABC}$ and $\log B = \log\rho_{AB} - \log\rho_B + \log\rho_{BC}$. It is easy to confirm that we get

$$-S(\rho_{ABC}) + S(\rho_{AB}) - S(\rho_B) + S(\rho_{BC}) \geq \mathrm{Tr}\,\{\rho_{ABC} - \exp(\log\rho_{AB} - \log\rho_B + \log\rho_{BC})\} \tag{4.89}$$

From Lieb's theorem we obtain

$$-S(\rho_{ABC}) + S(\rho_{AB}) - S(\rho_B) + S(\rho_{BC}) \geq \operatorname{Tr}\rho_{ABC} - \operatorname{Tr}\int_0^\infty \rho_{AB}\frac{1}{\rho_B + uI}\rho_{BC}\frac{1}{\rho_B + uI}\,du$$

$$= 1 - \operatorname{Tr}_B \int_0^\infty \rho_B \frac{1}{\rho_B + uI}\rho_B \frac{1}{\rho_B + uI}\,du \tag{4.90}$$

The integral can be evaluated with ease if we use the spectral decomposition of ρ_B and the completeness relation of its eigenvectors

$$\rho_B = \sum_i \lambda_i |u_i\rangle\langle u_i| \quad \text{and} \quad \frac{1}{\rho_B + uI} = \sum_i \frac{1}{\lambda_i + u}|u_i\rangle\langle u_i| \tag{4.91}$$

Then it follows

$$-S(\rho_{ABC}) + S(\rho_{AB}) - S(\rho_B) + S(\rho_{BC}) \geq 1 - \operatorname{Tr}\int_0^\infty du \sum_i \frac{\lambda_i^2}{(\lambda_i + u)^2}|u_i\rangle\langle u_i|$$

$$= 1 - \sum_i \lambda_i^2 \left[-\frac{1}{\lambda_i + u}\right]_0^\infty$$

$$= 1 - \sum_i \lambda_i = 0 \quad \blacksquare \tag{4.92}$$

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