Monogamy of Concurrence in Three-Qubit Systems

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Abstract

The concurrence is a measure of the entanglement between two quantum bits, related to the entanglement of formation between them. It has been found [3] that a monogamy is exhibited by concurrence in a three-qubit system. Thus, if there is an entangled system of three qubits A, B and C, the concurrence $\mathcal{C}_{AB}$ between A and B and the concurrence $\mathcal{C}_{AC}$ between A and C can not both be arbitrarily large. Following this, monogamy has been studied for other measures of quantum correlation and for more general systems. In this report, we review the definition of concurrence, its relation with entanglement of formation and mathematical expression for pure and mixed states, and the monogamy relation derived in Ref. [3].

Contents

Chapter 1

Entanglement of formation and concurrence

1.1 Introduction

Entanglement is a property of quantum systems which can not be explained by classical theory. A pure state of two or more systems (such as qubits) is called 'entangled' if it can not be expressed as a tensor product of individual one-qubit state vectors. Entangled systems show correlations that violate Bell inequalities predicted by classical theory, and they are also useful in procedures such as dense coding or quantum teleportation. This makes it important to study and quantify entanglement.

A pure state of two qubits A and B is 'separable', i.e. not entangled at all, if its state vector $|\Psi_{AB}\rangle$ is the tensor product of state vectors of the individual qubits, $|\Psi_{AB}\rangle = |\alpha_A\rangle \otimes |\beta_B\rangle$. Each of the qubits is in a pure state, and all information regarding it can be obtained by measuring it alone without using the other qubit. On the other hand, a state is 'maximally entangled' if the density operator of any one qubit (obtained by tracing the two-qubit density operator over the other qubit) is $\frac{1}{2}I$, such as the singlet state $\Psi^- = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$. For such a state, we can say that no useful information regarding any one of the qubits can be obtained unless one can operate on both the qubits together. In between these two extremes, we may have 'partially entangled' states such as $\cos(\theta)|\uparrow\downarrow\rangle + \sin(\theta)|\downarrow\uparrow\rangle$, where $0 \leq \theta \leq 2\pi$ and $\cos(\theta) \neq \sin(\theta)$. A partially entangled pair of qubits can be used for dense coding or teleportation, but with noise or with reduced fidelity [1].

Thus, we need to find a 'measure of entanglement'. It should ideally be 0 for a separable state, 1 for a maximally entangled state of two qubits, and a number between 0 and 1 for partially entangled states. It should also be invariant under local unitary operations and non-increasing under local non-unitary operations such as measurements, since it is known that such transformations can not increase entanglement [1, 2].

For pure states, one measure of entanglement is the 'entanglement of formation' of the system, defined as the Von Neumann entropy of any one of the single-qubit density operators:

$$E = S(\rho) = -\operatorname{tr}(\rho \log_2 \rho), \tag{1.1}$$

where ρ is ρ_A or ρ_B. We know that ρ_A and ρ_B have the same non-zero eigenvalues λ_i [7]. Thus we can write $E = -\sum_i \lambda_i \log_2 \lambda_i$, where we define $0 \log_2 0 = 0$. It has been shown in Ref. [1] that a system of N pairs of qubits, each with entanglement of formation E, can be converted to a system of a smaller number of singlets, where the number approaches

NE for large N. Also, since a unitary transformation operating on any one qubit can not change the density operator of the other qubit, clearly the entanglement of formation is unaffected. For a non-unitary transformation changing the initial bipartite pure state into a mixed state, the expected entanglement of formation will not increase, since E is a convex function of the density operators [1, 2].

1.2 Concurrence and its relation with the entanglement of formation

Now, let us consider a bipartite pure state $\Psi_{AB} = a|\uparrow\uparrow\rangle + b|\uparrow\downarrow\rangle + c|\downarrow\uparrow\rangle + d|\downarrow\downarrow\rangle$, $|a|^2 + |b|^2 + |c|^2 + |d|^2 = 1$. Taking the partial trace over B, the density operator ρ_A is

$$\rho_A = \mathrm{tr}_B \left|\Psi_{AB}\right\rangle \left\langle\Psi_{AB}\right| = \begin{pmatrix} |a|^2 + |c|^2 & ab^* + cd^* \\ a^*b + c^*d & |b|^2 + |d|^2 \end{pmatrix}, \tag{1.2}$$

expressed in the standard $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis. Its eigenvalues are

$$\lambda_{1,2} = \frac{1}{2} \pm \frac{1}{2}\sqrt{1 - 4\left|a\right|^2\left|d\right|^2 - 4\left|b\right|^2\left|c\right|^2 + 4(ab^*c^*d + a^*bcd^*)} = \frac{1}{2} \pm \frac{1}{2}\sqrt{1-\mathcal{C}^2}, \tag{1.3}$$

where $\mathcal{C} = 2\left|ad - bc\right|$. We see that $\lambda_1 + \lambda_2 = 1$ in this case. We take $\lambda_1 = x = \frac{1}{2}\left(1 + \sqrt{1-\mathcal{C}^2}\right)$, $\lambda_2 = 1 - x$.

Therefore, the entanglement of formation is

$$\begin{aligned} E(|\Psi_{AB}\rangle) &= -\,\mathrm{tr}(\rho \log_2 \rho) \\ &= -\sum_{i=1}^{2} \lambda_i \log_2 \lambda_i \\ &= -x\log_2 x - (1-x)\log_2(1-x) \\ &= h\left(\frac{1}{2}\left(1 + \sqrt{1-\mathcal{C}^2}\right)\right) \\ &= \mathcal{E}(\mathcal{C}), \end{aligned} \tag{1.4}$$

where $h(x) = x\log_2 x + (1-x)\log_2(1-x)$.

Thus we see that the entanglement of formation is a function of the quantity $\mathcal{C}$. Using the triangle and 'geometric mean $\leq$ arithmetic mean' inequalities, we get that

$$\begin{aligned} 2\left|ad - bc\right| &\leq 2(|ad| + |bc|) \\ &= 2\left(\sqrt{\left|a\right|^2\left|d\right|^2} + \sqrt{\left|b\right|^2\left|c\right|^2}\right) \\ &\leq 2\left(\frac{\left|a\right|^2 + \left|d\right|^2}{2} + \frac{\left|b\right|^2 + \left|c\right|^2}{2}\right) \\ &= \left|a\right|^2 + \left|d\right|^2 + \left|b\right|^2 + \left|c\right|^2 = 1. \end{aligned} \tag{1.5}$$

Hence, $0 \leq \mathcal{C} \leq 1$. It is easy to check that $\mathcal{C}$ is 0 for a separable state and 1 for a maximally entangled state such as a singlet. We also find that $\frac{1}{2}\left(1 + \sqrt{1-\mathcal{C}^2}\right)$ is a strictly decreasing function of $\mathcal{C}$ with range $\left[\frac{1}{2}, 1\right]$, and $h(x)$ restricted to the domain $\left[\frac{1}{2}, 1\right]$ is a strictly

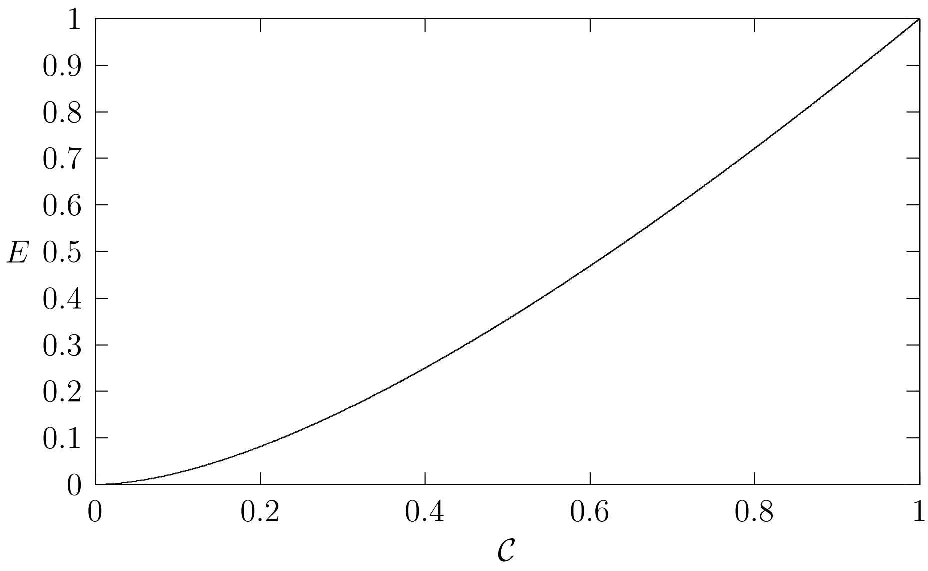

Figure 1.1: Plot of the entanglement of formation as a function of the concurrence

decreasing function of x. Hence, the entanglement of formation is a one-to-one strictly increasing function of the concurrence. Finally, we see that $\mathcal{E}(1) = 1$ and $\lim_{\mathcal{C}\to 0} \mathcal{E}(\mathcal{C}) = 0$. Thus, we take the quantity $\mathcal{C}$ as a measure of entanglement, and have given it the name 'concurrence' [9]. $\mathcal{C}$ has the advantage of having a simpler mathematical expression than E. We also mention here (without proof) that $\mathcal{E}$ ia a convex function, i.e. for two or more concurrences $\mathcal{C}_i$ with corresponding probabilities p_i, the average entanglement can not be less than than the entanglement function of the average concurrence: $\langle E\rangle \geq \mathcal{E}(\langle \mathcal{C}\rangle)$, where the average of a quantity is defined as $\langle q\rangle = \sum_i p_i q_i$. This will be helpful when finding the concurrence of a mixed state. However, entanglement of formation is a *concave* function of the *square* of the concurrence, and this fact will be used in proving the convexity of $\mathcal{C}^2$ as a function of the density operator, as well as in showing why there exists no monogamy relation for entanglement of formation. While the convexity has not been proved analytically in this report, they are apparent from the curvature of the graphs (Figs. 1.1 and 1.2).

In case of a bipartite pure state, we can also express the concurrence in terms of the density operator ρ_A of a subsystem instead of the individual coefficients. From the previously obtained expression of ρ_A, we get

$$\begin{aligned}
\det \rho_A &= \left(|a|^2 + |c|^2\right)\left(|b|^2 + |d|^2\right) - (ab^* + cd^*)(a^*b + c^*d) \\
&= |a|^2|b|^2 + |a|^2|d|^2 + |b|^2|c|^2 + |c|^2|d|^2 - (|a|^2|b|^2 + |c|^2|d|^2 + ab^*c^*d + a^*bcd^*) \\
&= |a|^2|d|^2 + |b|^2|c|^2 - ab^*c^*d - a^*bcd^* \\
&= (ad - bc)(a^*d^* - b^*c^*) \\
&= |ad - bc|^2 = \frac{\mathcal{C}^2}{4}. \qquad (1.6)
\end{aligned}$$

Thus, the concurrence of a bipartite pure state is $2\sqrt{\det \rho_A}$.

Yet another way to express the concurrence $\mathcal{C}$ in terms of the bipartite state vector $|\Psi_{AB}\rangle$ itself, which will be useful when considering the concurrence for mixed states, is using the "spin flip" transformation [8]. For a pure state of a single qubit $|\psi\rangle$, the spin

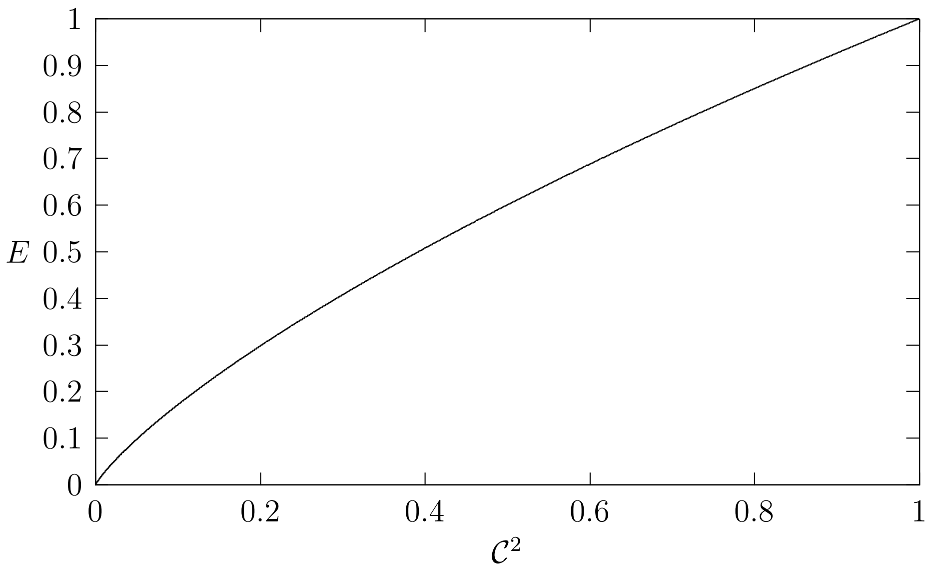

Figure 1.2: Plot of entanglement of formation as a function of the square of the concurrence

flipped state $\left|\tilde{\psi}\right\rangle$ is defined as

$$\left|\tilde{\psi}\right\rangle = \sigma_y|\psi^*\rangle, \tag{1.7}$$

where $|\psi^*\rangle$ is the complex conjugate of $|\psi\rangle$ when expressed in the standard basis $\{|\uparrow\rangle, |\downarrow\rangle\}$, and σ_y is the matrix $\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ when expressed in the same basis. (We have $\sigma_y|\uparrow\rangle = i|\downarrow\rangle$, $\sigma_y|\downarrow\rangle = -i|\uparrow\rangle$.) Spin-flip is an antilinear operator: if $|\phi\rangle = \sum_i c_i|b_i\rangle$, then $\left|\tilde{\phi}\right\rangle = \sum_i c_i^*\left|\tilde{b}_i\right\rangle$. For an n-qubit system, we apply the above transformation to each individual qubit. Thus, the spin-flipped state for a two-qubit pure state will be $\left|\tilde{\Psi}_{AB}\right\rangle = (\sigma_y \otimes \sigma_y)|\Psi^*_{AB}\rangle$, and the spin-flipped two-qubit density operator will be

$$\tilde{\rho} = (\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y). \tag{1.8}$$

For a general pure state of two qubits, $|\Psi_{AB}\rangle = a|\uparrow\uparrow\rangle + b|\uparrow\downarrow\rangle + c|\downarrow\uparrow\rangle + d|\downarrow\downarrow\rangle$, we have $\left|\tilde{\Psi}_{AB}\right\rangle = -a^*|\downarrow\downarrow\rangle + b^*|\downarrow\uparrow\rangle + c^*|\uparrow\downarrow\rangle - d^*|\uparrow\uparrow\rangle$. Thus, $\left\langle\tilde{\Psi}_{AB}\middle|\Psi_{AB}\right\rangle = -ad + bc + bc - ad = -2(ad - bc)$, and hence $\mathcal{C} = 2\,|ad - bc| = \left|\left\langle\tilde{\Psi}_{AB}\middle|\Psi_{AB}\right\rangle\right|$.

1.3 Entanglement of formation and concurrence of a bipartite mixed state

We now take take a *mixed* state ρ of two qubits A and B. A mixed state ρ of two qubits is said to be entangled if there exists no decomposition of ρ as an ensemble of separable pure states. Mixed-state entanglement is more complicated in some respect. For example, there exist entangled mixed states which do not violate any Bell inequality [2, 7].

For such a state, the entanglement of formation is defined in terms of the entanglements of the pure states in its decomposition [2, 8]. We take all possible pure-state decompositions of ρ, i.e. all ensembles of states $|\psi_i\rangle$ with probabilities p_i, such that $\rho = \sum_i p_i|\psi_i\rangle\langle\psi_i|$. The entanglement of formation is defined as before for each such pure state $|\psi_i\rangle$. For a particular ensemble, we can take the entanglement of formation to be the weighted average of the entanglements of the pure states in the ensemble. This has sometimes been called the 'entanglement of the ensemble' in this report for convenience, even though it has no physical significance. This average does not in general have the same value for every decomposition of the state ρ, e.g. the separable state $\frac{1}{4}I \otimes I$ can be written as an ensemble of maximally entangled states [7]. So the entanglement of formation of the state ρ is defined as the *minimum* value of this average over all possible ensemble decompositions of ρ:

$$E(\rho) = \min \sum_i p_i E(\psi_i). \tag{1.9}$$

It has been shown in Ref. [2] that E defined in this way can not be increased by local operations with classical communication. However, unlike for the pure case, the number of singlets such a state can be transformed into ('distilled') is less than E defined in this manner [2].

This definition of E is, however, difficult to work with, since it involves minimization over all ρ-ensembles. However, it has been shown [4, 8] that the entanglement of formation can be expressed in a simpler form. In the following paragraphs, we give the obtained expression of E, and then show the derivation of this expression as done in Ref. [8].

Let $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$ be the eigenvalues of the Hermitian matrix $\sqrt{\sqrt{\rho}\tilde{\rho}\sqrt{\rho}}$. They are also the square roots of the eigenvalues of the non-Hermitian matrix $\rho\tilde{\rho}$, because $\sqrt{\sqrt{\rho}\tilde{\rho}\sqrt{\rho}}|w_i\rangle = \lambda_i|w_i\rangle \implies \sqrt{\rho}\tilde{\rho}\sqrt{\rho}|w_i\rangle = \lambda_i^2|w_i\rangle$ and therefore $\rho\tilde{\rho}\left(\sqrt{\rho}|w_i\rangle\right) = \lambda_i^2\left(\sqrt{\rho}|w_i\rangle\right)$. We note that $\lambda_i \geq 0 \forall i$. In Ref. [8], it has been shown that the entanglement of formation is $E(\rho) = \mathcal{E}(\max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\})$, where the function $\mathcal{E}$ is defined as before. By comparison with the expression of entangement of formation of a pure state, we call $\max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}$ the *concurrence of the mixed state*, henceforth denoted by $\mathcal{C}(\rho)$.

Proving this involves two steps. We need to find a decomposition of ρ that gives the average entanglement equal to $\mathcal{E}(\mathcal{C}(\rho))$, and then prove that this is indeed the minimum value of entanglement for *any* decomposition of this state. But it is difficult to get to the correct decomposition directly. So we use the following property of ρ-ensembles obtained from the Schrödinger-HJW theorem [6]: For any two decompositions $\{|\psi_j\rangle, \alpha_j\}_{j=1}^n$ and $\{|\phi_i\rangle, \beta_i\}_{i=1}^m$ of ρ (i.e. $\rho = \sum_{j=1}^n \alpha_j|\psi_j\rangle\langle\psi_j| = \sum_{i=1}^m \beta_i|\phi_i\rangle\langle\phi_i|$), there exists a U-map from one to the other, i.e. there exists a set $\{U_{ij} \in \mathbb{C}|\sum_{j=1}^n U_{ji}^* U_{jk} = \delta_{ik}\}_{(j,k)=(1,1)}^{(m,n)}$, such that

$$\sqrt{\beta_i}|\phi_i\rangle = \sum_{j=1}^n U_{ij}\sqrt{\alpha_j}|\psi_j\rangle. \tag{1.10}$$

If $n = m$, then U is a unitary square matrix.

For the purpose of the proof, it is more convenient to absorb the factors into the state vectors, i.e. the vectors are 'subnormalized' such that $\langle\psi_j|\psi_j\rangle = \alpha_j$, $\langle\phi_i|\phi_i\rangle = \beta_j$. Then the decompositions simply become $\rho = \sum_{j=1}^n |\psi_j\rangle\langle\psi_j| = \sum_{i=1}^m |\phi_i\rangle\langle\phi_i|$, with the transformation

$$|\phi_i\rangle = \sum_{j=1}^n U_{ij}|\psi_j\rangle. \tag{1.11}$$

Conversely, if we have a subnormalized decomposition and apply the above transformation, the pure states in the transformed decomposition will be automatically subnormalized, with their inner products giving their probabilities in the ensemble [8]. This has been used in the derivation of bipartite mixed state entanglement. We start from a decomposition of ρ and perform a series of transformations, finally reaching the ensemble having entanglement $\mathcal{E}(\mathcal{C}(\rho))$.

Ensemble I: $|v_i\rangle$, the eigenvectors of ρ

The first ensemble taken is using the eigenvectors $|v_i\rangle,\ i = 1, \ldots, n \leq 4$ corresponding to the non-zero eigenvalues μ_i of ρ $[\rho|v_i\rangle = \mu_i|v_i\rangle,\ \mu_i > 0]$, subnormalized for convenience such that $\langle v_i|v_i\rangle = \mu_i$. Then we have $\rho = \sum_i |v_i\rangle\langle v_i|$.

Ensemble II: $\{|x_i\rangle\}$, satisfying $\langle\tilde{x}_i|x_j\rangle = \lambda_i\delta_{ij}$

Since the claimed expression of mixed state concurrence involves the numbers λ_i, it will be useful to consider an ensemble $\{|x_i\rangle\}_{i=1}^{n}$, where the pure states $|x_i\rangle$ satisfy

$$\langle\tilde{x}_i|x_j\rangle = \lambda_i\delta_{ij}. \tag{1.12}$$

As seen before, if such a decomposition exists, we must have a U-map from the $\{|v_j\rangle\}$ ensemble to the $\{|x_i\rangle\}$ ensemble, i.e. there must exist an $n \times n$ unitary matrix U such that

$$|x_i\rangle = \sum_j U_{ij}|v_j\rangle. \tag{1.13}$$

Then we have $|\tilde{x}_i\rangle = \sum_j U^*_{ij}|\tilde{v}_j\rangle$, and hence

$$\begin{aligned}\langle\tilde{x}_i|x_j\rangle &= \langle\tilde{v}_k|U_{ik}U_{jl}|v_l\rangle \\ &= U_{ik}\tau_{kl}\left(U^T\right)_{lj}\ \text{[Defining } \tau_{kl} = \langle\tilde{v}_k|v_l\rangle\text{]} \\ &= \left(U\tau U^T\right)_{ij}. \end{aligned} \tag{1.14}$$

τ is symmetric but not necessarily Hermitian. For the $|x_i\rangle$ vectors to satisfy the given condition, $U\tau U^T$ has to be diagonal, with diagonal entries λ_i. But it is a fact that for a symmetric matrix τ, there always exists a unitary U such that $U\tau U^T$ is diagonal with the diagonal entries real and non-negative [5]. To see that these diagonal entries are in fact the numbers λ_i, we note that they are the squares of the eigenvalues of $\tau\tau^*$. To verify this, let us take the diagonal entries of $U\tau U^T$ to be $\nu_i \geq 0$. Then we get $\left(U\tau U^T\right)_{il} = \sum_{j,k} U_{ij}\tau_{jk}U_{lk} = \nu_i\delta_{il}$. Also, U is unitary, which implies $\sum_j U^*_{ji}U_{jk} = \delta_{ik}$. Then we get

$$\begin{aligned}(U\tau\tau^*U^\dagger)_{im} &= \sum_{j,k,l} U_{ij}\tau_{jk}\tau^*_{kl}U^*_{ml} \\ &= \sum_{j,k,k',l} U_{ij}\tau_{jk'}\delta_{kk'}\tau^*_{kl}U^*_{ml} \\ &= \sum U_{ij}\tau_{jk'}U_{qk'}U^*_{qk}\tau^*_{kl}U^*_{ml}\ \left[\because \textstyle\sum_q U_{qk'}U^*_{qk} = \delta_{kk'}\right] \\ &= \sum \nu_i\delta_{iq}\nu_m\delta_{qm}\ [\because \nu_i \in \mathbb{R}] \\ &= \nu_i^2\delta_{im}. \end{aligned} \tag{1.15}$$

We find that $\tau\tau^*$ is diagonalized by U with diagonal entries ν_i^2. Thus, ν_i are the square roots of the eigenvalues of $\tau\tau^*$. Again, $\rho\tilde{\rho} = \sum_{k,l} (|v_k\rangle \langle v_l|) (|\tilde{v}_l\rangle \langle \tilde{v}_l|) = \sum_{k,l} \langle v_k|\tilde{v}_l\rangle |v_k\rangle \langle \tilde{v}_l|$, and hence in the $\{|\tilde{v}_i\rangle\}$ basis, $(\rho\tilde{\rho})_{ij} = \langle \tilde{v}_i| (\rho\tilde{\rho}) |\tilde{v}_j\rangle = \sum_k \langle \tilde{v}_i|v_k\rangle\langle v_k|\tilde{v}_j\rangle = \sum_k \tau_{ik}\tau^*_{kj} = (\tau\tau^*)_{ij}$ (since τ is symmetric). Therefore, $\rho\tilde{\rho}$ and $\tau\tau^*$ are the same matrix and have the same eigenvalues $\nu_i^2 = \lambda_i^2$. Thus, the diagonal entries of $U\tau U^T$ are nothing but the numbers λ_i, where they can be made to appear in the proper non-increasing order by choosing U accordingly. We have thus found a U-map from $\{|v_j\rangle\}$ to $\{|x_i\rangle\}$, where $\langle \tilde{x}_i|x_j\rangle = \lambda_i\delta_{ij}$.

Case A: $\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4 \geq 0$

Since the claimed expression involves the maximum of two terms, it would be helpful to take separate cases depending on which one is larger. We first consider the case where $\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4 \geq 0$. In this case, $\mathcal{C}(\rho) = \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4$.

Ensemble III: $\{|y_i\rangle\}$, with $|y_1\rangle = |x_1\rangle$, and $|y_j\rangle = i|x_j\rangle$ for other i

In the expression of concurrence, all terms except λ_1 have negative sign. This motivates the next decomposition of ρ, with the pure states $|y_i\rangle,\ i = 1, \dots, n$ chosen such that $|y_1\rangle = |x_1\rangle$, and $|y_j\rangle = i|x_j\rangle \forall j \neq 1$. This is physically equivalent to the first decomposition, but the phase factors change the signs in the expression of ensemble concurrence and lead to the following useful property of the ensemble.

The definition of concurrence involves taking the modulus, which is difficult to manipulate algebraically. Following Ref. [8], the 'preconcurrence' c of a pure (possibly subnormalized) state $|\psi\rangle$ is defined as

$$c(\psi) = \frac{\left\langle \tilde{\psi} \middle| \psi \right\rangle}{\langle \psi|\psi\rangle}, \tag{1.16}$$

i.e. the same expression as the concurrence without taking the absolute value, $\mathcal{C} = |c|$. Clearly, $\mathcal{C} = c$ if the preconcurrence is real and non-negative. Then the average preconcurrence of the $\{|y_i\rangle\}$ ensemble is found to be the quantity $\mathcal{C}(\rho)$ which we have claimed to be the state concurrence:

$$\begin{aligned} \langle c\rangle &= \sum_i \langle y_i|y_i\rangle \frac{\langle \tilde{y}_i|y_i\rangle}{\langle y_i|y_i\rangle} \\ &= \sum_i \langle \tilde{y}_i|y_i\rangle = \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4 = \mathcal{C}(\rho). \end{aligned} \tag{1.17}$$

Here we have used that if $n < 4$ then $\lambda_i = 0 \forall i > n$. This is the usefulness of this ensemble.

Ensemble IV: $\{|z_i\rangle\}$, where every $|z_i\rangle$ has the same concurrence

$\{y_i\}$ has the helpful property of having the average preconcurrence $\langle c\rangle = \mathcal{C}$. However, we have defined the *entanglement of formation*, and not the concurrence itself, as the ensemble average over the pure states, and so can not directly call $|\langle c\rangle|$ the concurrence of the ensemble. Hence, we need a decomposition where the preconcurrence of *every single* pure state is equal to $\mathcal{C}(\rho)$, because then we would certainly get the entanglement of formation of the ensemble to be $\mathcal{E}(\mathcal{C}(\rho))$, and hence will be justified in calling $\mathcal{C}(\rho)$ the ensemble concurrence.

The required ensemble $\{|z_i\rangle\}$ is once again related to $\{|y_i\rangle\}$ as $|z_i\rangle = \sum_{i=1}^{n} V_{ij}|y_j\rangle$ for $i = 1, \ldots, n$, where V is an $n \times n$ unitary matrix. The average preconcurrence of the ensemble $\{|z_i\rangle\}$ is

$$\langle c\rangle = \sum_i \langle \tilde{z}_i|z_i\rangle = \sum_i \left(VYV^T\right)_{ii} = \mathrm{tr}\left(VYV^T\right), \tag{1.18}$$

where Y is the real diagonal matrix defined as $Y_{ij} = \langle \tilde{y}_i|y_j\rangle$. This expression can be obtained the same way as the previously derived equation $\langle \tilde{x}_i|x_j\rangle = \left(U\tau U^T\right)_{ij}$. If V is real, we have $V^\dagger = V^T = V^{-1}$ and hence the trace is preserved. Thus any ensemble that can be obtained from the $\{|y_i\rangle\}$ ensemble using a *real* unitary matrix has the same preconcurrence as the $\{|y_i\rangle\}$ ensemble.

Among the ensembles obtained by real orthogonal matrices, let us try to obtain a decomposition where every pure state has the same preconcurrence. The procedure is as follows. First, we take the two states $|y_i\rangle$ with the smallest and largest values of the preconcurrence, say $|y_a\rangle$ and $|y_b\rangle$. Unless they all have the same preconcurrence to begin with, we will have $c(y_a) < \mathcal{C}(\rho)$ and $c(y_b) > \mathcal{C}(\rho)$. We now consider the group of all positive determinant real orthogonal transformations that act only on $|y_a\rangle$ and $|y_b\rangle$, leaving all the other states $|y_i\rangle$ unchanged ($|y_a\rangle \mapsto |z_a\rangle$, $|y_b\rangle \mapsto |z_b\rangle$, $|y_i\rangle \mapsto |y_i\rangle \forall i \neq a, b$). This group contains the identity transformation, as well as the transformation which simply interchanges these two states ($|z_a\rangle = |y_b\rangle$, $|z_b\rangle = |y_a\rangle$) and hence interchanges the concurrences. The set of transformations is a continuous group, and hence by continuity there must exist an intermediate transformation that makes $c(z_a) = \mathcal{C}(\rho)$. We perform this transformation, and keep repeating this procedure until we obtain a ρ-ensemble with all pure states having preconcurrence $\mathcal{C}(\rho)$. This we take to be our final decomposition $\{|z_i\rangle\}$, having average entanglement $\mathcal{E}(\mathcal{C}(\rho))$, with $\mathcal{C}(\rho)$ as defined before.

Proof of minimality

Now we need to show that this is indeed the *minimum* value of entanglement over all possible ensembles, i.e. no decomposition of ρ has a smaller average entanglement. For this, it suffices to show that no other decomposition has a smaller average *concurrence*, since the convexity and monotonicity of $\mathcal{E}$ implies that the average entanglement can not be less that the entanglement function of the average concurrence (If $\langle \mathcal{C}\rangle \geq \mathcal{C}(\rho)$ for any ensemble, then $\langle \mathcal{E}(\mathcal{C})\rangle \geq \mathcal{E}(\langle \mathcal{C}\rangle) \geq \mathcal{E}(\mathcal{C}(\rho))$). Now, the average concurrence of a general ensemble with $m \geq n$ state vectors is expressed similar to the average preconcurrence, but taking absolute values:

$$
\begin{aligned}
\langle\mathcal{C}\rangle &= \sum_i \left|\left(VYV^T\right)\right|_{ii} \\
&= \sum_i \left|\sum_{j,k} V_{ij} Y_{jk} V^T_{ji}\right| \\
&= \sum_i \left|\sum_j V_{ij} Y_{jj} V_{ij}\right| && \text{[Since } Y \text{ is diagonal]} \\
&= \sum_i \left|\sum_j \left(V_{ij}\right)^2 Y_{jj}\right|, \qquad (1.19)
\end{aligned}
$$

where $\sum_i V^*_{ij} V_{ij} = \sum_i \left|(V_{ij})^2\right| = 1 \forall j$. For convenience, let us denote $\left(V_{ij}\right)^2$ as α_{ij}. Without loss of generality, we can take each V_{i1} to be real, so that $\sum_i \alpha_{i1} = 1$. Then we can say

$$
\begin{aligned}
\sum_i \left|\sum_j \alpha_{ij} Y_{jj}\right| &\geq \left|\sum_{i,j} \alpha_{ij} Y_{jj}\right| \\
&= \left|\sum_i \alpha_{i1} Y_{11} + \sum_{i,j\geq 2} \alpha_{ij} Y_{jj}\right| \\
&= \left|\left(\sum_i \alpha_{i1}\right)\lambda_1 - \sum_{j=2}^{n}\left(\sum_i \alpha_{ij}\right)\lambda_j\right| \quad [\because Y_{11} = \lambda_1,\ Y_{jj} = -\lambda_j \forall j \geq 2] \\
&= \left|\lambda_1 - \sum_{j=2}^{n}\left(\sum_i \alpha_{ij}\right)\lambda_j\right| \\
&\geq \lambda_1 - \sum_{j=2}^{n}\left(\sum_i \left|\alpha_{ij}\right|\right)\lambda_j \\
&= \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4 = \mathcal{C}(\rho). \qquad (1.20)
\end{aligned}
$$

Thus, for a two-qubit density operator ρ, we get a decomposition for which the average entanglement of formation is $\mathcal{E}(\mathcal{C}(\rho))$, and no decomposition gives a lower value of entanglement. This proves the claim for $\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4 \geq 0$.

Case B: $\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4 < 0$

One case still remains to be considered, i.e. the case where $\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4 < 0$. For this case, the it is claimed that the entanglement is zero, i.e. the state ρ can be decomposed into unentangled pure states. To show this, we once again start with the decomposition $|x_i\rangle$, where $\langle\tilde{x}_i|x_j\rangle = \lambda_i \delta_{ij}$. In this case, we must have $n > 2$. If $n = 3$, we take $|x_4\rangle$ to be the zero vector.

For this case, we can always find phase factors θ_i such that $\sum_j e^{2i\theta_j}\lambda_j = 0$. We will give a geometric intuition to suggest why this is so. SInce we have four numbers $\lambda_i \geq 0$, where $\lambda_1 < \lambda_2 + \lambda_3 + \lambda_4$, we can always construct a quadrilateral whose sides have length λ_i (if $\lambda_4 = 0$, the side of that length is just a point, making the quadrilateral a triangle). While the quadrilateral $ABCDA$ may be constructed in several ways, one way is to construct a line segment $\overline{AB}$ of length λ_1, draw $\overline{AD}$ of length λ_4 with D lying on $\overline{AB}$, and then construct a triangle BCD with $\overline{BC} = \lambda_2$ and $\overline{CD} = \lambda_3$. Now, If we represent the vectors $\overrightarrow{AB}, \overrightarrow{BC}, \overrightarrow{CD}, \overrightarrow{DA}$ (whose sum is the zero vector) by the complex numbers $\zeta_1, \zeta_2, \zeta_3, \zeta_4$ respectively, then we get $\sum_j \zeta_j = 0$, where $|\zeta_j| = \lambda_j$, and $\arg \zeta_j$, defined by the angle the corresponding vector makes with the x-axis, is denoted by $2\theta_j$. Thus we get the above expression.

Now we define the decomposition $\{|z_i\rangle\}$ as $|z_i\rangle = \sum_i W_{ij}|x_j\rangle$, where W is the unitary matrix defined as

$$W = \frac{1}{2}\begin{pmatrix} e^{i\theta_1} & e^{i\theta_2} & e^{i\theta_3} & e^{i\theta_4} \\ e^{i\theta_1} & e^{i\theta_1} & -e^{i\theta_3} & -e^{i\theta_4} \\ e^{i\theta_1} & -e^{i\theta_2} & e^{i\theta_3} & -e^{i\theta_4} \\ e^{i\theta_1} & -e^{i\theta_2} & -e^{i\theta_3} & e^{i\theta_4} \end{pmatrix}. \tag{1.21}$$

Thus, $|z_i\rangle = \frac{1}{2}\sum_j \chi_{ij} e^{i\theta_j}|x_j\rangle$, where each χ_{ij} is either 1 or -1. The concurrence of each pure state $|z_i\rangle$ is found to be

$$\begin{aligned} \mathcal{C}(z_i) &= \langle z_i|\tilde{z}_i\rangle \\ &= \frac{1}{4}\sum_{j,k} \chi_{ij}\chi_{jk} e^{i\theta_j + i\theta_k}\langle x_j|\tilde{x}_k\rangle \\ &= \frac{1}{4}\sum_j (\chi_{ij})^2 e^{2i\theta_j}\lambda_j \\ &= 0. \end{aligned} \tag{1.22}$$

Hence, every state $|z_i\rangle$ has zero entanglement, which implies that a state with $\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4 < 0$ has zero entanglement of formation and zero concurrence. This proves our claim.

Here, we have followed Ref. [8] and done the entire analysis in the standard separable basis $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$. The problem could also be worked out in some other basis, such as the maximally entangled basis states. One particular basis that is often used [2, 4] is the so-called 'magic basis' $\{|e_i\rangle\}$:

$$|e_1\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle\right), \tag{1.23}$$

$$|e_2\rangle = \frac{i}{\sqrt{2}}\left(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle\right), \tag{1.24}$$

$$|e_3\rangle = \frac{i}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right), \tag{1.25}$$

$$|e_4\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right). \tag{1.26}$$

This basis has the advantage that $|\tilde{e}_i\rangle = -|e_i\rangle \forall i$, and hence the spin-flip transformation is simply complex conjugation with sign inversion when expressed in the magic basis [8]. So we have $\left|\tilde{\psi}\right\rangle = -|\psi^*\rangle_{\{|e_i\rangle\}} = -\sum_i \langle\psi|e_i\rangle|e_i\rangle$, the concurrence of a pure state $\Psi_{AB} = \sum_i \alpha_i|e_i\rangle$ is $\mathcal{C} = |\langle\Psi^*_{AB}|\Psi_{AB}\rangle| = |\sum_i \alpha_i^2|$, and the operator $\tilde{\rho}$ is simply ρ^* when expressed in the magic basis [4]. Here, we used the standard basis because this is the basis used in Ref. [3] when discussing monogamy of concurrence in the tripartite pure state. Also, the derivation of the expression for mixed state concurrence in the magic basis used more involved mathematics and was done only for the special case of two non-zero eigenvalues [4].

One property of concurrence that will be useful later is that $\mathcal{C}^2$ is a convex function of the density matrix ρ, i.e. if we have $\rho = \sum_i \alpha_i \rho_i$ with $0 \leq \alpha_i \leq 1 \forall i$ and $\sum_i \alpha_i = 1$, then $\mathcal{C}(\rho)^2 \leq \sum_i \alpha_i \mathcal{C}(\rho_i)^2$. This can be proved as follows. We first take the optimum decompositions (i.e. the decompositions giving the minimum average entanglement of formation) of ρ_i: $\rho_i = \sum_j p_{ij} |\psi_{ij}\rangle \langle\psi_{ij}| \forall i$. Then we have $E(\rho_i) = \mathcal{E}\left(\mathcal{C}(\rho_i)\right) = \sum_j p_{ij} E(\psi_{ij})$. Now, $\sum_{i,j} \alpha_i p_{ij} |\psi_{ij}\rangle \langle\psi_{ij}|$ is a decomposition of ρ, but it may not be the optimal decomposition. The average entanglement calculated for this decomposition is $\sum_{i,j} \alpha_i p_{ij} E(\psi_{ij}) = \sum_i \alpha_i E(\rho_i)$. Hence, the entanglement of formation of ρ will be $E(\rho) = \mathcal{E}(\mathcal{C}(\rho)) \leq \sum_i \alpha_i \mathcal{E}(\mathcal{C}(\rho_i))$. Now we use the property that entanglement of formation, though a convex function of $\mathcal{C}$, is a *concave* function of $\mathcal{C}^2$. Thus, $\sum_i \alpha_i \mathcal{E}(\mathcal{C}(\rho_i)) \leq \mathcal{E}\left(\sqrt{\sum_i \alpha_i \mathcal{C}(\rho_i)^2}\right)$. Therefore, $\mathcal{E}(\mathcal{C}(\rho)) \leq \mathcal{E}\left(\sqrt{\sum_i \alpha_i \mathcal{C}(\rho_i)^2}\right)$, and $\mathcal{E}$ being a strictly increasing function, this proves our claim.

Chapter 2

Concurrence in a tripartite pure state

We will now consider the case of a pure three-qubit system, and find the pair-wise concurrences and the relation between them. This chapter is a reworking of the derivation in Ref. [3]. For convenience, we will express the qubit basis states as $|0\rangle$ and $|1\rangle$, which may be considered to be equivalent to $|\uparrow\rangle$ and $|\downarrow\rangle$ respectively.

2.1 Monogamy inequality for squared concurrence

Let us now consider a pure state $|\xi\rangle$ of three qubits A, B and C. We first want to find the concurrence between A and B.

For a tripartite system, if we take any two of the qubits together (say A and B), then the two-qubit system is entangled to a single qubit (in this case, C). Hence the two-qubit density operator ρ_{AB} (obtained by taking the partial trace over C) has only two non-zero (positive) eigenvalues, and so does the product $\rho_{AB}\tilde{\rho}_{AB}$. Let the eigenvalues of $\rho_{AB}\tilde{\rho}_{AB}$ be λ_1^2 and λ_2^2. Then the concurrence will simply be $\mathcal{C}_{AB} = |\lambda_1 - \lambda_2|$. Then we see that

$$\begin{aligned} \mathcal{C}_{AB}^2 &= (\lambda_1 - \lambda_2)^2 = \lambda_1^2 + \lambda_2^2 - 2\lambda_1\lambda_2 \\ &= \mathrm{tr}(\rho_{AB}\tilde{\rho}_{AB}) - 2\lambda_1\lambda_2 \leq \mathrm{tr}(\rho_{AB}\tilde{\rho}_{AB}). \end{aligned} \tag{2.1}$$

Similarly, we can say that $\mathcal{C}_{AC}^2 \leq \mathrm{tr}(\rho_{AC}\tilde{\rho}_{AC})$. Adding them, we get the bound

$$\mathcal{C}_{AB}^2 + \mathcal{C}_{AC}^2 \leq \mathrm{tr}\,\rho_{AB}\tilde{\rho}_{AB} + \mathrm{tr}\,\rho_{AC}\tilde{\rho}_{AC}. \tag{2.2}$$

To evaluate the upper bound, i.e. the right hand side of this inequality, we need to express the three-qubit pure state in the standard basis $\{|ijk\rangle\}_{(i,j,k)=(0,0,0)}^{(1,1,1)}$:

$$|\xi\rangle = \sum_{i,j,k} a_{ijk}|ijk\rangle. \tag{2.3}$$

Then the density operator of the AB system will be

$$\begin{aligned} \rho_{AB} &= \mathrm{tr}_C(|\xi\rangle\langle\xi|) = \sum_k \langle k|\xi\rangle\langle\xi|k\rangle \\ &= \sum a_{ijk}a_{mnk}^*|ij\rangle\langle mn|, \end{aligned} \tag{2.4}$$

where the summation is over all indices. To avoid clutter, we will not use subscripts to denote subsystems unless necessary to avoid confusion. In everything that follows, the indices i and m will always be used to denote states of the qubit A; j and n for B; and k and p for C. The complex conjugate, ρ^*_{AB} is $\rho^*_{AB} = \sum a_{i'j'p} a^*_{m'n'p} |m'n'\rangle \langle i'j'|$. Thus, the operator $\tilde{\rho}_{AB}$ is obtained as

$$\begin{aligned}
\tilde{\rho}_{AB} &= (\sigma_y \otimes \sigma_y) \rho^*_{AB} (\sigma_y \otimes \sigma_y) \\
&= \sum \epsilon_{ab} \epsilon_{cd} |ac\rangle \langle bd| a_{i'j'p} a^*_{m'n'p} |m'n'\rangle \langle i'j'| \epsilon_{ef} \epsilon_{gh} |eg\rangle \langle fh| \\
&\text{[We define } \epsilon_{01} = -\epsilon_{10} = 1,\ \epsilon_{00} = \epsilon_{11} = 0.\ (\sigma_y)_{ab} = -i\epsilon_{ab}.] \\
&= \sum \epsilon_{ab} \epsilon_{cd} a_{i'j'p} a^*_{m'n'p} \epsilon_{ef} \epsilon_{gh} \langle bd|m'n'\rangle \langle i'j'|eg\rangle |ac\rangle \langle fh| \\
&= \sum \epsilon_{am'} \epsilon_{cn'} a_{i'j'p} a^*_{m'n'p} \epsilon_{i'f} \epsilon_{j'h} |ac\rangle \langle fh|.
\end{aligned} \tag{2.5}$$

Therefore,

$$\begin{aligned}
\rho_{AB} \tilde{\rho}_{AB} &= \sum a_{ijk} a^*_{mnk} |ij\rangle \langle mn| \epsilon_{am'} \epsilon_{cn'} a_{i'j'p} a^*_{m'n'p} \epsilon_{i'f} \epsilon_{j'h} |ac\rangle \langle fh| \\
&= \sum a_{ijk} a^*_{mnk} \epsilon_{am'} \epsilon_{cn'} a_{i'j'p} a^*_{m'n'p} \epsilon_{i'f} \epsilon_{j'h} \langle mn|ac\rangle |ij\rangle \langle fh| \\
&= \sum a_{ijk} a^*_{mnk} \epsilon_{mm'} \epsilon_{nn'} a_{i'j'p} a^*_{m'n'p} \epsilon_{i'f} \epsilon_{j'h} |ij\rangle \langle fh|,
\end{aligned} \tag{2.6}$$

and hence

$$\begin{aligned}
\mathrm{tr}(\rho_{AB} \tilde{\rho_{AB}}) &= \sum_{x,y} \langle xy| \rho_{AB} \tilde{\rho}_{AB} |xy\rangle \\
&= \sum a_{ijk} a^*_{mnk} \epsilon_{mm'} \epsilon_{nn'} a_{i'j'p} a^*_{m'n'p} \epsilon_{i'f} \epsilon_{j'h} \langle xy|ij\rangle \langle fh|xy\rangle \\
&= \sum a_{ijk} a^*_{mnk} \epsilon_{mm'} \epsilon_{nn'} a_{i'j'p} a^*_{m'n'p} \epsilon_{i'i} \epsilon_{j'j}.
\end{aligned} \tag{2.7}$$

Before further work with this expression, let us look at the single-qubit density operators. The density operator of A is given as $\rho_A = \sum a_{ijk} a^*_{mjk} |i\rangle \langle m|$. Its determinant is

$$\begin{aligned}
\det \rho_A &= (\rho_A)_{00} (\rho_A)_{11} - (\rho_A)_{01} (\rho_A)_{10} \\
&= \frac{1}{2} \sum (\rho_A)_{im} (\rho_A)_{i'm'} \epsilon_{ii'} \epsilon_{mm'} \\
&= \frac{1}{2} \sum a_{ijk} a^*_{mjk} a_{i'j'p} a_{m'j'p} \epsilon_{ii'} \epsilon_{mm'}.
\end{aligned} \tag{2.8}$$

We have $\rho_B = \sum a_{ijk} a^*_{ink} |j\rangle \langle n|$. Thus,

$$\begin{aligned}
\rho_B^2 &= \sum a_{ijk} a^*_{ink} |j\rangle \langle n| a_{i'j'p} a^*_{i'n'p} |j'\rangle \langle n'| \\
&= \sum a_{ijk} a^*_{ij'k} a_{i'j'p} a^*_{i'n'p} |j\rangle \langle n'| \\
\implies \mathrm{tr}(\rho_B^2) &= \sum a_{ijk} a^*_{ij'k} a_{i'j'p} a^*_{i'jp}
\end{aligned} \tag{2.9}$$

Similarly, $\mathrm{tr}(\rho_C^2) = \sum a_{ijk} a^*_{i'j'k} a^*_{ijp} a_{i'j'p}$.

Now we use the identity $\epsilon_{nn'} \epsilon_{j'j} = \delta_{nj'} \delta n' j - \delta_{nj} \delta_{n'j'}$, and the corresponding identity for $\epsilon_{mm'}\epsilon_{i'i}$, in the obtained expression for $\mathrm{tr}(\rho_{AB}\tilde{\rho}_{AB})$:

$$\begin{aligned}
\mathrm{tr}(\rho_{AB}\tilde{\rho}_{AB}) &= \sum a_{ijk}a^*_{mnk}a^*_{m'n'p}a_{i'j'p}\epsilon_{mm'}\epsilon_{i'i}(\delta_{nj'}\delta_{n'j} - \delta_{nj}\delta_{n'j'}) \\
&= \sum a_{ijk}a^*_{mj'k}a^*_{m'jp}a_{i'j'p}(\delta_{mi'}\delta_{m'i} - \delta_{mi}\delta_{m'i'}) \\
&- \sum a_{ijk}a^*_{mjk}a^*_{m'j'p}a_{i'j'p}\epsilon_{mm'}(-\epsilon_{ii'}) \\
&= \sum a_{ijk}a^*_{i'j'k}a^*_{ijp}a_{i'j'p} - \sum a_{ijk}a^*_{ij'k}a^*_{i'jp}a_{i'j'p} + 2\det\rho_A \\
&= 2\det\rho_A - \mathrm{tr}(\rho_B^2) + \mathrm{tr}(\rho_C^2).
\end{aligned} \tag{2.10}$$

We can further simplify the expression, using the fact that the density operators have unit trace. Thus, for any two-dimensional density operator ρ, we have

$$\begin{aligned}
\mathrm{tr}(\rho^2) &= \sum_{i,j}\rho_{ij}\rho_{ji} \\
&= \sum_i \rho_{ii}^2 + \sum_{i\neq j}\rho_{ij}\rho_{ji} \\
&= \sum_i \rho_{ii}^2 + \sum_{i\neq j}\rho_{ii}\rho_{jj} - \sum_{i\neq j}\rho_{ii}\rho_{jj} + \sum_{i\neq j}\rho_{ij}\rho_{ji} \\
&= \sum_{i,j}\rho_{ii}\rho_{jj} - 2(\rho_{11}\rho_{22} - \rho_{12}\rho_{21}) \\
&= (\mathrm{tr}\,\rho)^2 - 2\det\rho \\
&= 1 - 2\det\rho.
\end{aligned} \tag{2.11}$$

Thus we may write

$$\mathrm{tr}(\rho_{AB}\tilde{\rho}_{AB}) = 2(\det\rho_A + \det\rho_B - \det\rho_C). \tag{2.12}$$

By symmetry, we must also have

$$\mathrm{tr}(\rho_{AC}\tilde{\rho}_{AC}) = 2(\det\rho_A + \det\rho_C - \det\rho_B). \tag{2.13}$$

Adding the two equations, we get $\mathrm{tr}(\rho_{AB}\tilde{\rho}_{AB})+\mathrm{tr}(\rho_{AC}\tilde{\rho}_{AC}) = 4\det\rho_A$, and thus we finally get the inequality

$$\mathcal{C}_{AB}^2 + \mathcal{C}_{AC}^2 \leq 4\det\rho_A. \tag{2.14}$$

The right hand side of this inequality can be physically interpreted as follows. We can think of the pair BC as a single system entangled with A. Even though BC has a 4-dimensional Hilbert space, since it is entangled with the qubit A, only two basis vectors are required to express the pure state $|\xi\rangle$ (the eigenvectors of ρ_{BC} corresponding to non-zero eigenvalues). If we the consider $|\xi\rangle$ to be a bipartite state of two qubits, the concurrence between A and BC can be written as $\mathcal{C}_{A(BC)} = 2\sqrt{\det\rho_A}$, as we have seen in the previous chapter. Thus we can write

$$\mathcal{C}_{AB}^2 + \mathcal{C}_{AC}^2 \leq \mathcal{C}_{A(BC)}^2. \tag{2.15}$$

This relation has been interpreted as follows [3]. The separate entanglements of A with the qubits B and C is bounded by the entanglement of A with BC as a whole, and the entanglement used up between A with B (as measured by the squared concurrence) is not available for C. If A is highly entangled with B, its entanglement with C must be low. This is called a monogamy relation (the word 'monogamy' means being married to one person at a time).

Throughout this chapter, we will be dealing with the square of the concurrence as a measure of entanglement, rather than the concurrence itself. In fact, the squared concurrence has sometimes been given the name 'tangle', represented by τ (as in Ref. [9] and the arXiv preprint of Ref. [3]). Here, we will stick to writing in terms of the concurrence, since that is the more prevalent usage.

2.2 Monogamy inequality for a tripartite mixed state

Let us now consider the case of a tripartite mixed state. In that case, all four dimensions of the Hilbert space of BC may be involved, and hence we can not regard BC as analogous to a qubit and define $\mathcal{C}^2_{A(BC)}$. But a related quantity $\left(\mathcal{C}^2_{A(BC)}\right)^{\min}$ may be defined, in a way analogous to the definition of the entanglement of formation of a mixed state. We consider all possible pure state decompositions of ρ, i.e. all sets $\{(\psi_i \in \mathcal{H}_{ABC}, p_i \in (0,1))\}$ such that $\rho = \sum_i p_i |\psi_i\rangle \langle\psi_i|$. For each such ρ-ensemble, we can define the squared concurrence as a weighted average of the squared concurrences of the pure states: $\left\langle \mathcal{C}^2_{A(BC)} \right\rangle = \sum_i p_i \mathcal{C}_{A(BC)}(\psi_i)^2$. Then we define $\left(\mathcal{C}^2_{A(BC)}\right)^{\min}$ as the minimum of this average over all possible ρ-ensembles,

$$\left(\mathcal{C}^2_{A(BC)}\right)^{\min} = \min \left\langle \mathcal{C}^2_{A(BC)} \right\rangle = \min_{\{\psi_i, p_i\}} \sum_i p_i \mathcal{C}_{A(BC)}(\psi_i)^2. \tag{2.16}$$

Then we see that the analogue of the previously derived inequality holds for mixed states:

$$\mathcal{C}^2_{AB} + \mathcal{C}^2_{AC} \leq (\mathcal{C}^2_{A(BC)})^{\min} \tag{2.17}$$

. To prove this, we consider the pure states $|\psi_i\rangle$ of an optimal ρ-ensemble, i.e. one that minimizes $\left\langle \mathcal{C}^2_{A(BC)} \right\rangle$. Then we can write the inequality for pure states for each such state and take the average, getting

$$\left\langle \mathcal{C}_{AB}(\rho)^2 \right\rangle_{\langle\rho\rangle = \rho_{AB}} + \left\langle \mathcal{C}_{AC}(\rho)^2 \right\rangle_{\langle\rho\rangle = \rho_{AC}} \leq \min \left\langle \mathcal{C}_{A(BC)} \right\rangle = \left(\mathcal{C}^2_{A(BC)}\right)^{\min}. \tag{2.18}$$

The right hand side of the inequality gives $(\mathcal{C}^2_{A(BC)})^{\min}$. On the left hand side, we have two terms: the average squared concurrence between A and B over a set of mixed states whose average is ρ_{AB}, and the average of the squared concurrence between A and C over a set of mixed states whose average is ρ_{AC}. But it has been shown before that the squared concurrence is a convex function over the set of density matrices, i.e. for an ensemble of density operators, we have $\mathcal{C}(\langle\rho\rangle)^2 \leq \langle\mathcal{C}(\rho)^2\rangle$. Therefore, we get the inequality for tripartite mixed states,

$$\mathcal{C}_{AB}(\rho_{AB})^2 + \mathcal{C}_{AC}(\rho_{AC})^2 \leq \left\langle \mathcal{C}_{AB}(\rho)^2 \right\rangle_{\langle\rho\rangle = \rho_{AB}} + \left\langle \mathcal{C}_{AC}(\rho)^2 \right\rangle_{\langle\rho\rangle = \rho_{AC}} \leq \left(\mathcal{C}^2_{A(BC)}\right)^{\min}. \tag{2.19}$$

2.3 Possibility of similar inequalities for other entanglement measures

Let us now continue with our discussion on pure states of three qubits. We now want to see if there can be tighter inequalities of this form based on other measures of entanglement.

To investigate this matter, we first note that for every set of values of $\mathcal{C}^2_{AB}$, $\mathcal{C}^2_{AC}$ and $\mathcal{C}^2_{A(BC)}$ in $[0,1]$ satisfying the equality $\mathcal{C}^2_{AB}+\mathcal{C}^2_{AC}=\mathcal{C}^2_{A(BC)}$, there exists a state of three qubits having the said values of the concurrences. To show this, we consider the following pure state of ABC [3]:

$$|\phi\rangle=\alpha|100\rangle+\beta|010\rangle+\gamma|001\rangle,\ |\alpha|^2+|\beta|^2+|\gamma|^2=1. \tag{2.20}$$

Then we have the density matrix

$$\begin{aligned}\rho_{AB}&=(\alpha|10\rangle+\beta|01\rangle)(\alpha^*\langle 10|+\beta^*\langle 01|)+|\gamma|^2|00\rangle\langle 00|\\&=|\alpha|^2|10\rangle\langle 10|+\alpha\beta^*|10\rangle\langle 01|+\alpha^*\beta|01\rangle\langle 10|+|\beta|^2|01\rangle\langle 01|+|\gamma|^2|00\rangle\langle 00|\\&=\begin{pmatrix}|\gamma|^2&0&0&0\\0&|\beta|^2&\alpha^*\beta&0\\0&\alpha\beta^*&|\alpha|^2&0\\0&0&0&0\end{pmatrix},\end{aligned} \tag{2.21}$$

when expressed in the standard basis.

Thus we have $\tilde{\rho}=\begin{pmatrix}0&0&0&0\\0&|\alpha|^2&\alpha^*\beta&0\\0&\alpha\beta^*&|\beta|^2&0\\0&0&0&|\gamma|^2\end{pmatrix}$, and hence

$$\rho\tilde{\rho}=\begin{pmatrix}0&0&0&0\\0&2|\alpha\beta|^2&2|\beta|^2\alpha^*\beta&0\\0&2|\alpha|^2\alpha\beta^*&2|\alpha\beta|^2&0\\0&0&0&0\end{pmatrix}, \tag{2.22}$$

with eigenvalues 0 and $4|\alpha\beta|^2$. Thus we have $\mathcal{C}^2_{AB}=4|\alpha\beta|^2$. Similarly, $\mathcal{C}^2_{AC}=4|\alpha\gamma|^2$ and $\mathcal{C}_{A(BC)}=4\det\rho_A=4|\alpha|^2\left(|\beta|^2+|\gamma|^2\right)$. Hence we see that for any value of the concurrences satisfying the inequality, we can get a state $|\phi\rangle$ consistent with those values by choosing the coefficients α, β and γ accordingly.

Now let $\Gamma(\mathcal{C})$ be a monotonically increasing function of $\mathcal{C}$ that may be treated as an alternative measure of entanglement. For simplicity we assume $\Gamma(0)=0$ and $\Gamma(1)=1$. Suppose Γ exhibits an inequality analogous to the one for concurrence, $\Gamma^2_{AB}+\Gamma^2_{AC}\le\Gamma^2_{A(BC)}$. From the above example, we see that for any two non-negative x and y satisfying $x^2+y^2\le 1$, we can have a pure state of ABC with $\mathcal{C}_{AB}=x$, $\mathcal{C}_{AC}=y$ and $\mathcal{C}_{A(BC)}=\sqrt{x^2+y^2}$. Therefore, Γ will satisfy such an inequality only if $\Gamma(x)^2+\Gamma(y)^2\le\Gamma(\sqrt{x^2+y^2})^2$ for all such x and y. (If we write Γ as a function of the *squared* concurrence, $\Gamma(\mathcal{C})=\mathcal{G}(\mathcal{C}^2)$, then the property can be written as $\mathcal{G}(x^2)+\mathcal{G}(y^2)\le\mathcal{G}(x^2+y^2)$. Entanglement of formation is a function of concurrence, but it satisfies no such inequality because it is a concave function of the squared concurrence.) For such a Γ, could there exist a sate for which $\Gamma^2_{AB}+\Gamma^2_{AC}=\Gamma^2_{A(BC)}$ but $\mathcal{C}^2_{AB}+\mathcal{C}^2_{AC}<\mathcal{C}^2_{A(BC)}$, suggesting that Γ gives a more stringent bound? We see that this is not possible, because if $\mathcal{C}^2_{AB}+\mathcal{C}^2_{AC}<\mathcal{C}^2_{A(BC)}$, then $\Gamma^2_{AB}+\Gamma^2_{AC}=\Gamma(\mathcal{C}_{AB})^2+\Gamma(\mathcal{C}_{AC})^2\le\Gamma\left(\sqrt{\mathcal{C}^2_{AB}+\mathcal{C}^2_{AC}}\right)^2<\Gamma(\mathcal{C}_{A(BC)})^2=\Gamma^2_{A(BC)}$. On the other hand, states giving an equality for concurrence will also give an equality for Γ only if $\Gamma=\mathcal{C}$. Thus, among all functions of $\mathcal{C}$, $\mathcal{C}$ itself is the optimal measure of entanglement with respect to this inequality. There may, however, be other optimal measures of entanglement which are not functions of $\mathcal{C}$.

2.4 Residual entanglement

We now study the *difference* between the two sides of the concurrence inequality. This may be interpreted as the amount of entanglement between A and BC that *can not* be accounted for by the pair-wise entanglements. We will refer to it as the 'residual entanglement'. Let us once again consider ABC to be in a pure state $|\xi\rangle = \sum_{i,j,k} a_{ijk}|ijk\rangle$. We define λ_1^{AB} and λ_2^{AB} to be the square roots of the two eigenvalues of $\rho_{AB}\tilde{\rho}_{AB}$, and λ_1^{AC} and λ_2^{AC} are defined similarly. We have seen before that $\mathcal{C}_{AB}^2 = \mathrm{tr}\,(\rho_{AB}\tilde{\rho}_{AB}) - 2\lambda_1^{AB}\lambda_2^{AC}$, and a similar expression can be derived for $\mathcal{C}_{AC}^2$. Also, we have seen that $\mathrm{tr}\,(\rho_{AB}\tilde{\rho}_{AB}) + \mathrm{tr}\,(\rho_{AC}\tilde{\rho}_{AC}) = 4\det(\rho_A) = \mathcal{C}_{A(BC)}^2$. Therefore, we get

$$\mathcal{C}_{A(BC)}^2 - \mathcal{C}_{AB}^2 - \mathcal{C}_{AC}^2 = 2\lambda_1^{AB}\lambda_2^{AB} + 2\lambda_1^{AC}\lambda_2^{AC}. \tag{2.23}$$

Now we will derive an expression for the residual entanglement in terms of the coefficients a_{ijk}.

We first study the product $\lambda_1^{AB}\lambda_2^{AB}$. $\rho_{AB}\tilde{\rho}_{AB}$ is an operator acting on the 4-dimensional space $\mathcal{H}_{AB}$, with eigenvalues $(\lambda_1^{AB})^2$, $(\lambda_2^{AB})^2$, 0 and 0. Thus $\lambda_1^{AB}\lambda_2^{AB}$ is the square root of the determinant of the transformation obtained by restricting the domain on $\rho_{AB}\tilde{\rho}_{AB}$ to its range. As we have seen before, $\rho_{AB} = \sum a_{ijk}a^*_{mnk}|ij\rangle\langle mn| = (\sum a_{ijk}|ij\rangle)(\sum a^*_{mnk}\langle mn|) = \sum_k |v_k\rangle\langle v_k|$, where $|v_k\rangle = \sum a_{ijk}|ij\rangle$ for $k = 0, 1$. Then $\rho\tilde{\rho} = \sum_{i,j}\langle v_i|\tilde{v_j}\rangle|v_i\rangle\langle\tilde{v_j}|$ has its range spanned by $|v_0\rangle$ and $|v_1\rangle$. If we now have a matrix R such that $\rho_{AB}\tilde{\rho}_{AB}|v_l\rangle = \sum_i R_{kl}|v_k\rangle$, then we can sat that $\lambda_1^{AB}\lambda_2^{AB} = \sqrt{\det R}$. We have

$$\begin{aligned}
\rho_{AB}\tilde{\rho}_{AB}|v_l\rangle &= \sum a_{ijk}a^*_{mnk}\epsilon_{mm'}\epsilon_{nn'}a_{i'j'p}a^*_{m'n'p}\epsilon_{i'f}\epsilon_{j'h}|ij\rangle\langle fh|a_{stl}|st\rangle \\
&= \sum a_{ijk}a^*_{mnk}\epsilon_{mm'}\epsilon_{nn'}a_{i'j'p}a_{m'n'p}\epsilon_{i'f}\epsilon_{j'h}a_{fhl}|ij\rangle \\
&= \sum a^*_{mnk}\epsilon_{mm'}\epsilon_{nn'}a_{i'j'p}a^*_{m'n'p}\epsilon_{i'f}\epsilon_{j'h}a_{fhl}|vk\rangle.
\end{aligned} \tag{2.24}$$

So it is seen that $R_{kl} = \sum a_{fhl}a^*_{mnk}\epsilon_{mm'}\epsilon_{nn'}a^*_{m'n'p}a_{i'j'p}\epsilon_{i'f}\epsilon_{j'h}$. Finding the square toot of its determinant involves tedious algebra, but it has been found [3] that the expression is symmetric under swapping any two qubits. Thus we find that the residual entanglement can be considered to be the 'three-way tangle' of the system, denoted in Ref. [3] as τ_{ABC} and invariant under permutation of qubits. Thus we can write

$$\mathcal{C}_{A(BC)}^2 = \mathcal{C}_{AB}^2 + \mathcal{C}_{AC}^2 + \tau_{ABC}. \tag{2.25}$$

This may be interpreted in the following manner. The entanglement between A and the system BC is consists of the entanglements of A with the individual qubits B and C, as well as the entanglement τ_{ABC} shared between all three qubits.

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