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UNIVERSITY OF CALIFORNIA, SAN DIEGO

**Semi-Algebraic Entanglement Consistency Relations:
Fundamental and Dynamical**

A dissertation submitted in partial satisfaction of the
requirements for the degree
Doctor of Philosophy

in

Physics

by

Grant Warren Allen

Committee in charge:

Professor David Meyer, Chair
Professor Daniel Arovas, Co-Chair
Professor Julio Barreiro
Professor John McGreevy
Professor Nolan Wallach

2017

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The dissertation of Grant Warren Allen is approved, and it is acceptable in quality and form for publication on microfilm and electronically:

Co-Chair

Chair

University of California, San Diego

2017

EPIGRAPH

*Correlations have physical reality;
that which they correlate does not.*

—N. David Mermin [1]

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Less directly, but in fact, more significantly to the completion of this work — thank you to my family and friends. Oh and even students. You all helped shape the ship that held together long enough for my arrival here.

Chapter 2, in part, is currently being prepared for submission for publication of the material as, G. W. Allen, O. Bucicovschi, and D. A. Meyer, “Entanglement Constraints on States Locally Connected to the Greenberger-Horne-Zeilinger State.” The dissertation

author is a primary investigator and author of this paper.

Chapter 3, in large part, is a reprint of the material as it appears in G. W. Allen and D. A. Meyer, “Polynomial Monogamy Relations for Entanglement Negativity,” *Phys. Rev. Lett.* 118, 080402 (2017). The dissertation author was a primary investigator and author of this paper.

Chapter 4, in part, is currently being prepared for submission for publication of the material as, G. W. Allen, O. Bucicovschi, and D. A. Meyer, “Another Comparison of Entanglement Measures Negativity and Concurrence.” The dissertation author is a primary investigator and author of this paper.

Chapter 5, in part, is currently being prepared for submission for publication of the material as, G. W. Allen and D. A. Meyer, “Complex Entanglement Constraints under Simple Dynamics: Ising, Toffoli, and Fredkin.” The dissertation author is a primary investigator and author of this paper.

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G. W. Allen, O. Bucicovschi and D. A. Meyer, “Another Comparison of Entanglement Measures Negativity and Concurrence,” preparing for publication.

G. W. Allen, O. Bucicovschi and D. A. Meyer, “Entanglement Constraints on States Locally Connected to the Greenberger-Horne-Zeilinger State,” preparing for publication.

G. W. Allen and D. A. Meyer, “Polynomial Monogamy Relations for Entanglement Negativity,” Phys. Rev. Lett. **118**, 080402 (2017).

M. W. Coffey and G. W. Allen, “Eigenvalue degeneracy relations for a fully connected isotropic spin network,” J. Phys. A: Math Theor. **44**, 395303 (2011).

ABSTRACT OF THE DISSERTATION

**Semi-Algebraic Entanglement Consistency Relations:
Fundamental and Dynamical**

by

Grant Warren Allen

Doctor of Philosophy in Physics

University of California, San Diego, 2017

Professor David Meyer, Chair
Professor Daniel Arovas, Co-Chair

Encoding the state of physical systems, the many-body wavefunction lives in a Hilbert space that conveniently offers a tensor factor to each constituent of the system. Consequentially, the wavefunction inherits structural properties such as entanglement, a new type of quantum correlation across the tensor factors. Entanglement can be quantified by forming polynomials in the wavefunction that remain invariant under local operations, which in turn naturally imply the properties we intuit about entanglement. It follows from the Tarski-Seidenberg theorem that these polynomial entanglement

measures must obey polynomial constraints. It is among these constraints that the core features separating quantum correlations from classical correlations are illuminated, such as their monogamous nature. The smallest non-trivial system which exhibits entanglement monogamy tradeoffs governed by polynomial constraints is three qubits, for which we find novel constraints that are stronger than the previously known constraints, and which may as well be a complete description of three-qubit entanglement since the number of degrees of freedom matches the number of entanglement measures. A remarkable redundancy known in three qubits is that any party's total entanglement decomposes exactly into bipartite and tripartite type entanglement; we find that this behavior is merely part of the GHZ family tradition, and that any party within the n -qubit GHZ SLOCC equivalence class also has total entanglement which decomposes exactly into all k -partite type entanglements, thus providing insight into strong versions of monogamy relations. Refocusing back to tripartite systems, we then suppose arbitrarily many degrees of freedom into our subsystems, which appear to refuse all temptations of polygamy. Up to this point we have only been considering idealized isolated systems as it is known that monogamy relations aren't sensitive to the total purity, however we then find entanglement constraints which are violated by globally mixed states, ultimately suggesting that environments can enable entanglement to grow beyond what is otherwise allowed. Finally, we address the dynamical behavior of entanglement under several key interactions, and characterize the couplings according to their ability to generate entanglement.

Chapter 1

Introduction and Preliminaries

The program of quantifying nature is a remarkably valuable endeavor, allowing one to explore properties of physical systems *abstractly* and predict their behavior whereas even upon discovering inconsistencies in the abstraction often leads to new insight into the physical world. Examples include Maxwell’s unification of light and electromagnetism, Einstein’s amelioration of Newtonian physics with electromagnetism, Planck’s resolution of black-body spectra, and Bell’s inequality with the ensuing Bell test experiments. The latter is particularly relevant to this dissertation, as it demonstrated the existence of *quantum correlations*.

In modern times, it is often repeated that quantum correlations, such as entanglement, are the powerhouse of quantum technologies — a phrase which has practically become the slogan of quantum information theory. If quantum correlations are indeed somehow the cause of anything unusual or spooky arising in quantum mechanics, then monogamy laws are the puppet masters which tame them, quantitatively speaking — this work attempts to push the envelope of such entanglement constraints to its limit. In large part, we will require a fair amount of algebraic calculation unfamiliar to the common physicist, so much so that it seems a one-line summary of this dissertation could be, if

quantum mechanics is just linear algebra, then quantum correlations is just polynomial algebra. After giving a brief overview of this dissertation, the rest of the introductory chapter is meant as a short exposition of entanglement measures and the mathematical trickery that permeates the calculations of subsequent chapters.

Following the introduction, Chapter 2 will start off examining the smallest non-trivial system where entanglement constraints can exist — three quantum bits. A common idea in the field is that the entanglement can come in incommensurable types, such as GHZ-type and W-type entanglement, an idea which has its origins in three qubits by taking the quotient of Hilbert space by local matrices from the special linear group. It would be misleading to just say that entanglement comes in different types, since in fact almost all three-qubit states have GHZ-type entanglement and the states with W-type entanglement occupy zero volume in Hilbert space. Therefore we might expect to be able to understand all three-qubit entanglement by looking at states which are locally equivalent to the GHZ state. Like magic, we find that the GHZ state possesses tangles, a family of related entanglement measures, with rather elegant transformation properties under stochastic local operations. These transformation properties allow us to parametrize all the possible tangles, bipartite and tripartite. Then, by applying some algebraic techniques, we describe the structure of the allowed tangles with a single inequality. This new constraint turns out to be strictly stronger than the monogamy relation, and also turns out to imply the familiar marginal eigenvalue inequality. We then use the tangle transformation properties of the n -qubit GHZ state to reveal that even in the n -qubit GHZ equivalence class, the total entanglement of any party decomposes exactly into all k -partite type entanglement — a direct generalization of three-qubit behavior known as strong monogamy. We finally summarize our results into a framework that explains why entanglement is constrained by polynomials in the first place.

In Chapter 3, we consider whether monogamy is an artifact of limited systems,

which is to say, qubits. In order to quantify in a tractable way the entanglement in systems with more degrees of freedom, we use a different entanglement measure than before which is not a polynomial invariant although it is still semi-algebraic — the entanglement negativity. First we find the exact constraints for negativity in three qubits, which turn out to be new to the literature. We then generalize the states which saturate the inequality, to conjecture the constraints for systems with arbitrarily many degrees of freedom, for which numerical experimentations have not lead to any counterexamples. So while not an entirely rigorous result, our suspicions about monogamy violations in these systems have been minimized.

In Chapter 4, we re-examine three qubits, this time allowing for classical correlations *via* impure states. The constraints we find for either the negativity or the tangle for pure three-qubit states can be violated with mixed three-qubit states. Recall that the original monogamy relation was proved on pure states, and because of the simplicity of the expression, it was almost trivial to generalize to mixed states. Therefore the monogamy relation is insensitive to the purity of the state, yet our constraints can be violated by mixed states. We find a family of states which violate pure state constraints in a significant enough way that no other numerical experimentation of ours has gone beyond, therefore we conjecture an algebraic expression for the constraints on arbitrary mixed states of three qubits.

At last in Chapter 5, we take inspiration from Ilya Prigogine and Isabelle Stengers' description of statistical phenomena in Newtonian physics [2], "From the point of view of dynamics, collisions and correlations play an equivalent roll." From that, we decide to explore the behavior of entanglement during the dynamics of some fundamental interactions. In particular we are interested in how entanglement arises due to interactions, so we look at the set of all states which evolved from zero entanglement, *e.g.*, product states, which we coin the concrescence. We map the concrescence into the space of

tangles which allows us compare with previous results, and we suggest taking the ratio of volume of the image of the concrescence with the volume of the image of Hilbert space as an ordering on the interactions based on their ability to generate entanglement.

1.1 Entanglement Measures

Let's begin with a perhaps under-appreciated yet vastly general theorem of Verstraete *et al.* [3].

Theorem: *A linearly homogeneous non-negative function of a pure state, i.e., $M(\alpha\rho) = |\alpha|M(\rho) \geq 0$, with $\rho^2 = \rho, \alpha \in \mathbb{C}$, that is invariant under local $SL(N, \mathbb{C})$ matrices where N is the dimension of a tensor factor, is an entanglement monotone.*

Proof: We repeat the arguments of Verstraete *et al.*, here for convenience. The monotonicity condition is the following,

$$M(\rho) \geq \text{Tr}(A\rho A^\dagger)M\left(\frac{A\rho A^\dagger}{\text{Tr}(A\rho A^\dagger)}\right) + \text{Tr}(\bar{A}\rho\bar{A}^\dagger)M\left(\frac{\bar{A}\rho\bar{A}^\dagger}{\text{Tr}(\bar{A}\rho\bar{A}^\dagger)}\right), \quad (1.1)$$

where $A, \bar{A}$ act locally on one tensor factor, and $A^\dagger A + \bar{A}^\dagger \bar{A} = I_N$, so $A, \bar{A}$ do not necessarily have unit determinant, and N is the dimension of the tensor factor that $A, \bar{A}$ act on. Now using the assumption of the theorem, the traces obviously cancel, due to homogeneity of M ,

$$M(\rho) \geq M(A\rho A^\dagger) + M(\bar{A}\rho\bar{A}^\dagger). \quad (1.2)$$

Now we can stick in a determinant to make the matrices inside M have unit determinants,

$$\begin{aligned} M(\rho) &\geq |\det(A)|^{2/N} M\left(\frac{A\rho A^\dagger}{|\det(A)|^{2/N}}\right) + |\det(\bar{A})|^{2/N} M\left(\frac{\bar{A}\rho\bar{A}^\dagger}{|\det(\bar{A})|^{2/N}}\right) \\ &= \left(|\det(A)|^{2/N} + |\det(\bar{A})|^{2/N}\right) M(\rho), \end{aligned} \quad (1.3)$$

where the coefficient can be simplified with, $|\det(A)|^{2/N} = |\det(A^\dagger A)|^{1/N}$, which is the geometric mean of the eigenvalues of $A^\dagger A$. The geometric mean is never greater than the arithmetic mean, so we get,

$$\left(|\det(A^\dagger A)|^{1/N} + |\det(\bar{A}^\dagger \bar{A})|^{1/N}\right) \leq \frac{1}{N} \text{Tr}(A^\dagger A) + \frac{1}{N} \text{Tr}(\bar{A}^\dagger \bar{A}) = \frac{1}{N} \text{Tr}(I_N) = 1, \quad (1.4)$$

which makes the monotonicity condition hold, completing the proof. $\square$

The above theorem is for functions defined on pure states. A function's domain can be extended to mixed states, by extending the function linearly on the pure state decompositions. Since pure state decompositions are not unique, typically one looks for the extrema, where the minimum is called the convex roof, and the maximum is called the concave roof,

$$\begin{aligned} \check{M}(\rho) &= \inf \sum_i p_i M(|\psi_i\rangle), \\ \hat{M}(\rho) &= \sup \sum_i p_i M(|\psi_i\rangle), \end{aligned} \quad (1.5)$$

where a check will mean convex roof and a hat will mean concave roof and the inf/sup are over all possible pure state decompositions $\{p_i, \psi_i\}$ of ρ .

We'd like to state another very important theorem, but first it might be useful to unpack the ideas of the convex/concave roof with a toy example inspired by Uhlmann [4]. Consider the set of states for a pure rebit (a qubit with real coefficients),

$$|\psi\rangle = \cos(\theta/2) |0\rangle + \sin(\theta/2) |1\rangle, \quad (1.6)$$

with $\theta \in [0, 2\pi]$ so that this set has the structure of a 1-sphere. The mixed states of a rebit are convex combinations of pure rebit states, and thus are structurally equivalent to the

2-ball. Now consider the toy function on *pure* rebit states,

$$\mathcal{M}(|\psi\rangle) = |\langle 0|\psi\rangle \langle \psi|1\rangle|, \quad (1.7)$$

which will be extended to the mixed states via the convex roof, $\check{\mathcal{M}}$ and the concave roof $\hat{\mathcal{M}}$. Note that the average $\mathcal{M}$ on *any* decomposition will be referred to as a roof point, so a convex roof point is the infimum roof point, and a concave roof point is the supremum roof point. To visualize this, let the state space be a disk on a plane, and the value of the function $\mathcal{M}$ be the height — so far, only $\mathcal{M}$ is explicitly known on the pure states (the boundary), see Fig. 1.1 where the point $\rho = \begin{pmatrix} 0.45 & -0.25 \\ -0.25 & 0.55 \end{pmatrix}$ is drawn in the yellow disk floor as a blue point, and directly vertical to it, a single roof point is drawn in as a purple point, and the black straight line shows that the roof point is indeed obtained as an average of two values on the boundary.

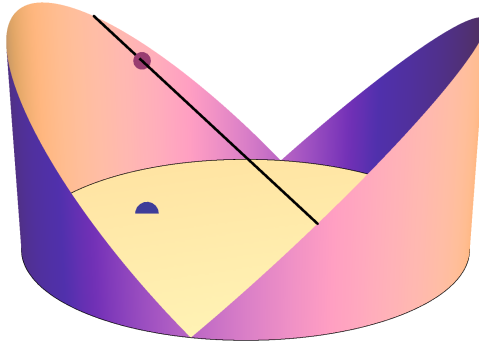


Figure 1.1: Bloch disk for a rebit with $\mathcal{M}$ defined on the pure states, and a roof point for a state ρ .

The extremization process to find the convex/concave roof is typically a very difficult calculation, but our low dimensional example makes the process quite feasible. See Fig. 1.2 which shows the locus of roof points, the purple line, arising from the many ways of decomposing ρ into pure states, the red lines show two decompositions which achieve the max and min. Note that the decomposition which extremizes the roof is

called the optimal decomposition and it is not necessarily unique.

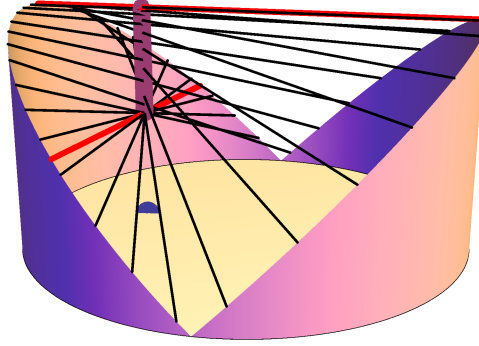


Figure 1.2: The locus of roof points for a state ρ .

Repeating the process for all states will give a surface that coincides with the boundary walls, see Fig. 1.3 for both the convex and concave roof. Generally speaking, the convex roof is the maximal convex function that coincides with the wall, and the concave roof is the minimal concave function that coincides with the wall (which appears to be the opposite convention used by architectures).

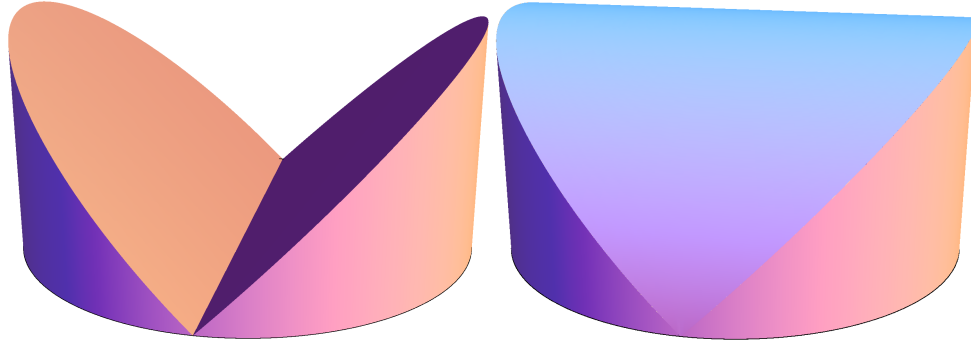


Figure 1.3: The convex roof, $\check{\mathcal{M}}$, (left). The concave roof, $\hat{\mathcal{M}}$, (right).

Some roof points have the following property, that for *some* decomposition of ρ ,

$$\mathcal{M}(\{p_i, \psi_i\}) = \sum_i p_i \mathcal{M}(|\psi_i\rangle) = \mathcal{M}(|\psi_i\rangle) \quad \forall i, \quad (1.8)$$

and these roof points are called flat roof points. If for some function, the convex roof points are all flat roof points, then that function's convex roof extension is also called flat.

Flat convex roofs have the useful property that,

$$f(\check{\mathcal{G}}(\rho)) = \check{f}(\mathcal{G}(\rho)), \quad (1.9)$$

where $\mathcal{G}$ is some flat roof, and f is any function that preserves the convexity over the state space, so that taking the convex roof extension commutes with composition. Our toy example is clearly flat (take decompositions that make chords parallel to the chord that goes from the two zeros of the wall). As an example, consider taking the convex roof extension of $\mathcal{M}^2$ — Fig. 1.4 shows two decompositions which achieve the convex roof point at ρ for $\mathcal{M}$ where one of the decompositions obeys the flatness property — then the roof points are shown for $\mathcal{M}^2$ for the *same* decompositions of ρ , which clearly no longer overlap, however the decomposition with the flatness property remains the optimal decomposition, producing the convex roof point.

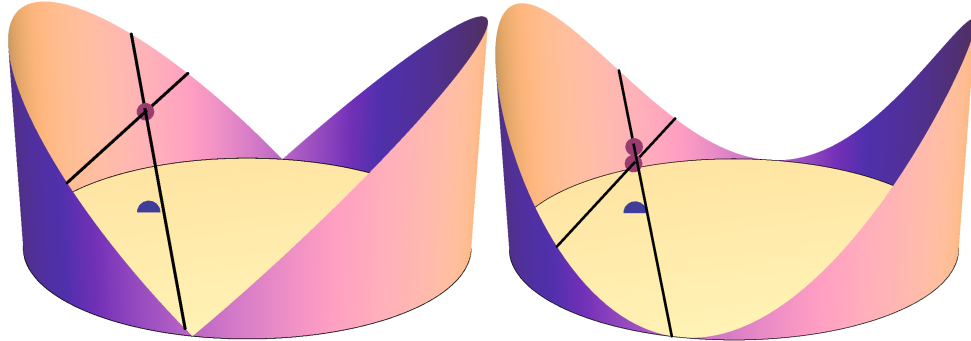


Figure 1.4: Coincident convex roof points of $\mathcal{M}$ separate for $\mathcal{M}^2$, the flat decomposition continues to produce the convex roof point of $\mathcal{M}^2$.

The above example is particularly important because it turns out that a common entanglement measure, the tangle, has a flat convex roof extension, yet the squared tangle appears so often in expressions — but as demonstrated, it is not necessary to consider the differences of the squared convex roof tangle and the convex roof squared tangle. Furthermore, as Uhlmann [4] showed, all convex roofs based off expectation values of anti-linear Hermitian operators are flat, and the k -tangles which we will use in Chapter 2,

fit this criteria.

There is one more property about roofs worth emphasizing. The number of pure states which make up a particular decomposition of ρ is called the length of the decomposition. Consider a different toy function defined on pure states as,

$$\mathcal{S}(|\psi\rangle) = \sin^2(5 \langle 0|\psi\rangle \langle \psi|1\rangle), \quad (1.10)$$

and we will try to find the convex roof point for the state $\rho = \begin{pmatrix} 0.65 & 0.15 \\ 0.15 & 0.35 \end{pmatrix}$. The left of Fig. 1.5 shows the locus of roof points in green obtained by checking all of the decompositions of length two for the blue point ρ . As the right of Fig. 1.5 shows, one can achieve a lesser roof point by consider decompositions of length three, with the convex roof point shown in purple. This shows that an explicit minimization, even in low dimensions can be quite complicated. In any case, the example shows the importance of

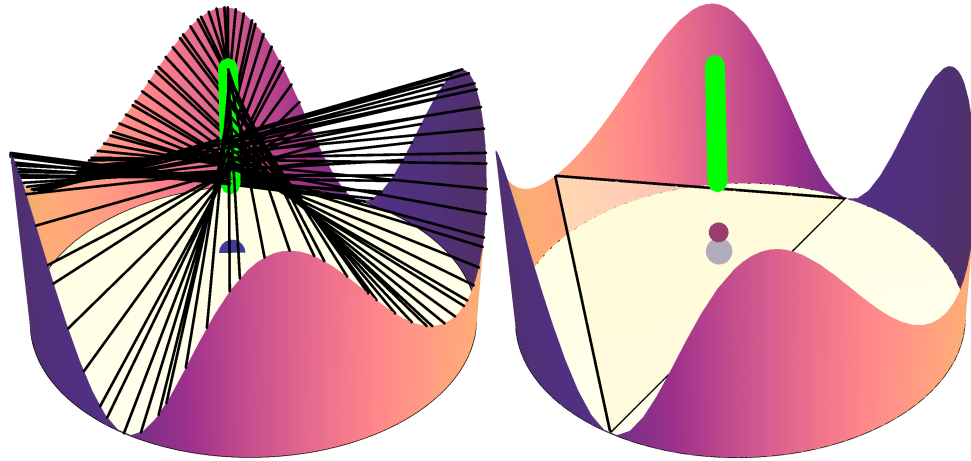


Figure 1.5: The locus of roof points for decompositions of length two (left). A decomposition of length three achieves the convex roof point (right).

Carathéodory's theorem, which states that a point ρ in a convex subset of $\mathbb{R}^d$ needs no longer than a decomposition of length $d + 1$ — this can significantly simplify the search for optimal decompositions. Also note, Hughston, Jozsa, and Wootters showed that all

decompositions are connected by unitary matrices [5] which then can parametrize all the decompositions for explicit minimizaion. And finally, for confirming intuition, Fig. 1.6 shows the convex and concave roofs of $\mathcal{S}$, note that the convex roof is not flat, but the concave roof is.

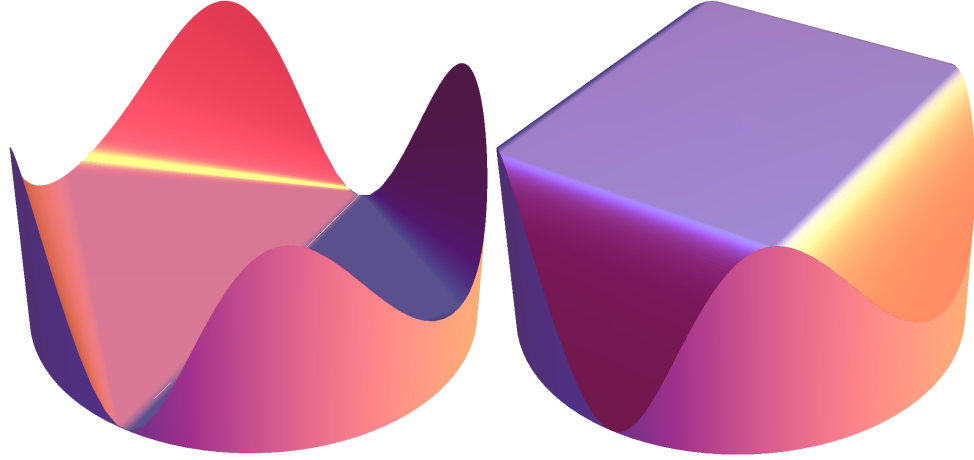


Figure 1.6: The convex roof, $\check{\mathcal{S}}$, (left). The concave roof, $\hat{\mathcal{S}}$, (right).

Now we are perhaps ready to state the final (also seemingly under-appreciated and highly useful) theorem for this section, which comes from Tajima [6].

Theorem: Consider a linearly homogeneous non-negative function, M , of a pure state, i.e., $M(\alpha|\psi\rangle\langle\psi|) = |\alpha|M(|\psi\rangle\langle\psi|) \geq 0$, with $\alpha \in \mathbb{C}$ that is invariant under local $SL(2, \mathbb{C})$ operations, which can be expressed as the condition, $M\left(\frac{A|\psi\rangle\langle\psi|A^\dagger}{\text{Tr}(A|\psi\rangle\langle\psi|A^\dagger)}\right) = \frac{|\det(A)|}{\text{Tr}(A|\psi\rangle\langle\psi|A^\dagger)}M(|\psi\rangle\langle\psi|)$ for a local $A \in GL(2, \mathbb{C})$ where 2 is the dimension of a tensor factor. The convex roof extension of M satisfies, $\check{M}\left(\frac{A\rho A^\dagger}{\text{Tr}(A\rho A^\dagger)}\right) = \frac{|\det(A)|}{\text{Tr}(A\rho A^\dagger)}\check{M}(\rho)$.

Proof: We follow a similar line of arguments as Tajima, although the same arguments have also appeared earlier by Horodecki *et al.* [7]. Under the local stochastic map A , define σ such that, $\rho \mapsto \sigma = \frac{1}{\text{Tr}(A\rho A^\dagger)}A\rho A^\dagger$. Now define two possibly different pure state decompositions of ρ , $\{p_i, |\psi_i\rangle\}$ and $\{p_i^*, |\psi_i^*\rangle\}$, where the starred decomposition is the optimal decomposition for $\check{M}$. Similarly define two possibly different pure state decompositions of σ , $\{q_i, |\phi_i\rangle\}$ and $\{q_i^*, |\phi_i^*\rangle\}$. These decompositions are connected in

the following sense,

$$\begin{aligned} \{p_i, |\psi_i\rangle\} &\xleftarrow{A^{-1}} \{q_i^*, |\phi_i^*\rangle\}, \\ \{p_i^*, |\psi_i^*\rangle\} &\xrightarrow{A} \{q_i, |\phi_i\rangle\}, \end{aligned} \quad (1.11)$$

with the explicit relations,

$$\begin{aligned} |\phi_i\rangle &= \frac{A |\psi_i^*\rangle}{\sqrt{\text{Tr}(A |\psi_i^*\rangle \langle \psi_i^*| A^\dagger)}}, \\ q_i &= p_i^* \frac{\text{Tr}(A |\psi_i^*\rangle \langle \psi_i^*| A^\dagger)}{\text{Tr}(A \rho A^\dagger)}, \end{aligned} \quad (1.12)$$

and

$$\begin{aligned} |\psi_i\rangle &= \frac{A^{-1} |\phi_i^*\rangle}{\sqrt{\text{Tr}(A^{-1} |\phi_i^*\rangle \langle \phi_i^*| A^{-\dagger})}}, \\ p_i &= q_i^* \text{Tr}(A^{-1} |\phi_i^*\rangle \langle \phi_i^*| A^{-\dagger}) \text{Tr}(A \rho A^\dagger). \end{aligned} \quad (1.13)$$

Notice how the roof points are connected,

$$\begin{aligned} M(\{q_i, |\phi_i\rangle\}) &= \sum_i q_i M(|\phi_i\rangle \langle \phi_i|) \\ &= \sum_i p_i^* \frac{\text{Tr}(A |\psi_i^*\rangle \langle \psi_i^*| A^\dagger)}{\text{Tr}(A \rho A^\dagger)} M\left(\frac{A |\psi_i^*\rangle \langle \psi_i^*| A^\dagger}{\text{Tr}(A |\psi_i^*\rangle \langle \psi_i^*| A^\dagger)}\right) \\ &= \sum_i p_i^* \frac{|\det(A)|}{\text{Tr}(A \rho A^\dagger)} M(|\psi_i^*\rangle \langle \psi_i^*|) \\ &= \frac{|\det(A)|}{\text{Tr}(A \rho A^\dagger)} M(\{p_i^*, |\psi_i^*\rangle\}), \end{aligned} \quad (1.14)$$

and an analogous relation holds with the other pair of decompositions (just move the

star). Now consider the following,

$$\begin{aligned}
\check{M}(\sigma) &= M(\{q_i^*, |\phi_i^*\rangle\}) \\
&= \frac{|\det(A)|}{\text{Tr}(A\rho A^\dagger)} M(\{p_i, |\psi_i\rangle\}) \\
&\geq \frac{|\det(A)|}{\text{Tr}(A\rho A^\dagger)} M(\{p_i^*, |\psi_i^*\rangle\}) \\
&= \frac{|\det(A)|}{\text{Tr}(A\rho A^\dagger)} \check{M}(\rho),
\end{aligned} \tag{1.15}$$

where the inequality follow from the fact that the roof point $M(\{p_i, |\psi_i\rangle\})$ must be greater than or equal to the convex roof point $M(\{p_i^*, |\psi_i^*\rangle\})$. On the other hand,

$$\begin{aligned}
\check{M}(\sigma) &= M(\{q_i^*, |\phi_i^*\rangle\}) \\
&\leq M(\{q_i, |\phi_i\rangle\}) \\
&= \frac{|\det(A)|}{\text{Tr}(A\rho A^\dagger)} M(\{p_i^*, |\psi_i^*\rangle\}) \\
&= \frac{|\det(A)|}{\text{Tr}(A\rho A^\dagger)} \check{M}(\rho).
\end{aligned} \tag{1.16}$$

Thus, $\frac{|\det(A)|}{\text{Tr}(A\rho A^\dagger)} \check{M}(\rho) \leq \check{M}(\sigma) \leq \frac{|\det(A)|}{\text{Tr}(A\rho A^\dagger)} \check{M}(\rho)$ and the theorem is proved. $\square$

Note how useful this theorem is — if you know the value of $\check{M}$ for one particular state, then you can easily calculate $\check{M}$ on *any* state that is locally stochastically connected to it without having to explicitly evaluate the infimum — and it is this fact that is heavily exploited in Chapter 2. One can actually go back to the first theorem, and replace M with $\check{M}$, and the exact same argument shows that $\check{M}$ is monotonic on mixed states. It is thus tempting to call the theorems of this section the fundamental theorems of SLOCC monotones.

1.2 Elimination Theory

Since we are almost exclusively working with polynomial invariants, it is useful to review some of the mathematical tricks involved when dealing with polynomials, namely the resultant, Gröbner bases, and the cylindrical decomposition. For the resultant [8], consider two univariate polynomials of degree N and M respectively,

$$\begin{aligned} p(x) &= \sum_{i=-\infty}^{\infty} p_i x^i, \\ q(x) &= \sum_{i=-\infty}^{\infty} q_i x^i, \end{aligned} \tag{1.17}$$

where we define $p_i = q_i = 0$ if $i < 0$, $p_i = 0$ if $i > N$, and $q_i = 0$ if $i > M$. Suppose you want to know whether the two polynomials share a common zero. Form the Sylvester matrix, R , with elements,

$$\begin{aligned} R_{i,j} &= p_{i-j}, & 0 \leq i \leq M+N-1, & 0 \leq j \leq M-1, \\ R_{i,j} &= q_{i-j+M}, & 0 \leq i \leq M+N-1, & M \leq j \leq M+N-1, \end{aligned} \tag{1.18}$$

so that the first M columns are the coefficients of p shifted downwards once each column, and the last N columns are the coefficients of q shifted downwards once each column. The resultant with respect to x of p and q , is defined as the determinant of R ,

$$\text{Res}_x(p, q) = \det(R), \tag{1.19}$$

which vanishes if and only if p and q share a common zero. The resultant gives a condition for simultaneous zeros if the coefficients are in a field — so we can let the coefficients themselves be variables, and the resultant can therefore eliminate a variable from two equations without explicitly solving for it.

Let's compute an example to see how this works in practice. Consider a parametriza-

tion of the familiar Möbius strip in $\mathbb{R}^3$,

$$\begin{aligned} x(v, u) &= \left(1 + \frac{v}{2} \cos(u)\right) \cos(2u), \\ y(v, u) &= \left(1 + \frac{v}{2} \cos(u)\right) \sin(2u), \\ z(v, u) &= \frac{v}{2} \sin(u), \end{aligned} \tag{1.20}$$

with $-1 \leq v \leq 1$, and $0 \leq u \leq \pi$. We will turn the parametric surface into an implicit surface using resultants to eliminate the parameters. To simplify the process, we will transform the above into an algebraic parametrization, using some trigonometric formulas to simplify,

$$\begin{aligned} x(v, c) &= \left(1 + \frac{v}{2}c\right)(2c^2 - 1), \\ y(v, c) &= \left(1 + \frac{v}{2}c\right)2c\sqrt{1 - c^2}, \\ z(v, c) &= \frac{v}{2}\sqrt{1 - c^2}, \end{aligned} \tag{1.21}$$

where $c = \cos(u)$ which is now treated as an independent parameter, with $-1 \leq v \leq 1$, and $-1 \leq c \leq 1$. We will additionally square away the square root, and define new polynomials,

$$\begin{aligned} f_1 &= 1 + x + \frac{v}{2}c - 2c^2 - vc^3, \\ f_2 &= y^2 - 4c^2 - 4vc^3 + (4 - v^2)c^4 + 4vc^5 + v^2c^6, \\ f_3 &= z^2 - \frac{v^2}{4} + \frac{v^2}{4}c^2, \end{aligned} \tag{1.22}$$

so that the zeros of the f_i 's will give the parametrization from above. We first eliminate c from f_1 and f_2 by computing the resultant since we want both f_i 's to simultaneously

vanish,

$$\begin{aligned}
 g_1 &= \text{Res}_c(f_1, f_2) \\
 &= \det \begin{pmatrix}
 1+x & \cdot & \cdot & \cdot & \cdot & \cdot & y^2 & \cdot & \cdot \\
 \frac{v}{2} & 1+x & \cdot & \cdot & \cdot & \cdot & 0 & y^2 & \cdot \\
 -2 & \frac{v}{2} & 1+x & \cdot & \cdot & \cdot & -4 & 0 & y^2 \\
 -v & -2 & \frac{v}{2} & 1+x & \cdot & \cdot & -4v & -4 & 0 \\
 \cdot & -v & -2 & \frac{v}{2} & 1+x & \cdot & 4-v^2 & -4v & -4 \\
 \cdot & \cdot & -v & -2 & \frac{v}{2} & \cdot & 4v & 4-v^2 & -4v \\
 \cdot & \cdot & \cdot & -v & -2 & \frac{v}{2} & v^2 & 4v & 4-v^2 \\
 \cdot & \cdot & \cdot & \cdot & -v & -2 & \cdot & v^2 & 4v \\
 \cdot & \cdot & \cdot & \cdot & \cdot & -v & \cdot & \cdot & v^2
 \end{pmatrix} \\
 &= \frac{1}{64} v^6 (64x^2 - 16v^2x^2 - 32v^2x^3 - 128x^4 - 16v^2x^4 + 64x^6 + 64y^2 - 16v^2y^2 + v^4y^2 \\
 &\quad - 32v^2xy^2 - 256x^2y^2 - 32v^2x^2y^2 + 192x^4y^2 - 128y^4 - 16v^2y^4 + 192x^2y^4 + 64y^6).
 \end{aligned} \tag{1.23}$$

Of course, we prefer to use software instead, see Fig. 1.7.

```

In[1]:= f1 = 1 - 2 c^2 +  $\frac{c v}{2}$  - c^3 v + x;
        f2 = -4 c^2 + 4 c^4 - 4 c^3 v + 4 c^5 v - c^4 v^2 + c^6 v^2 + y^2;
        Resultant[f1, f2, c] // Factor

Out[3]=  $\frac{1}{64} v^6 (64 x^2 - 16 v^2 x^2 - 32 v^2 x^3 - 128 x^4 - 16 v^2 x^4 + 64 x^6 + 64 y^2 - 16 v^2 y^2 + v^4 y^2 -$ 
         $32 v^2 x y^2 - 256 x^2 y^2 - 32 v^2 x^2 y^2 + 192 x^4 y^2 - 128 y^4 - 16 v^2 y^4 + 192 x^2 y^4 + 64 y^6)$ 

```

Figure 1.7: Resultants in Mathematica.

The resultant of f_1 and f_3 is,

$$g_2 = \text{Res}_c(f_1, f_3) = \frac{-1}{256}v^2(-4v^4 + v^6 + 8v^4x - 4v^4x^2 + 64v^2z^2 - 20v^4z^2 - 64v^2xz^2 - 256z^4 + 128v^2z^4 - 256z^6). \quad (1.24)$$

To make $g_1 = g_2 = 0$, we are not interested in the case where $v = 0$, so we will drop this trivial factor. Now we eliminate v from g_1, g_2 with another resultant,

$$\begin{aligned} \text{Res}_v\left(\frac{g_1}{v^6}, \frac{g_2}{v^2}\right) &= \frac{1}{68719476736}(-y + x^2y + y^3 - 2xz - 2x^2z - 2y^2z + yz^2)^2 \\ &\quad \times (-y + x^2y + y^3 + 2xz + 2x^2z + 2y^2z + yz^2)^2 (\cdots 97 \text{ terms } \cdots)^2. \end{aligned} \quad (1.25)$$

Of the 3 polynomial factors, the first gives the implicit surface we've been seeking. See Fig 1.8 for the solution set to the polynomial equation, $-y + x^2y + y^3 - 2xz - 2x^2z - 2y^2z + yz^2 = 0$, with the parametrized Möbius strip.

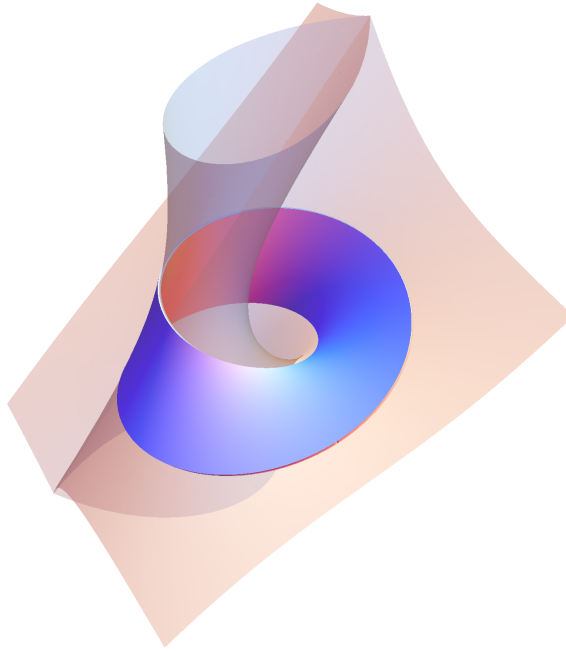


Figure 1.8: A Möbius strip and the algebraic variety in which it lives.

A recurring theme from our polynomial adventures is that it is not always obvious which factors are important, and which are ok to drop— we'll just have to be careful. The resultant tends to shine when one is eliminating a small number of variables, and when more variables need eliminating, the resultant can become cumbersome.

Another useful notion is the Gröbner basis [9]. Given a set of n polynomials, $F = \{f_1, \dots, f_n\}$, there exists another set of m polynomials $G = \{g_1, \dots, g_m\}$, such that any linear combination of the f_i 's with polynomial coefficients has zero remainder after polynomial division by G . The set G is called the Gröbner basis for the ideal generated by F . There are several algorithms for computing a Gröbner basis, the most straight forward may be the Buchberger algorithm. The idea is that you take every polynomial in F and divide every other polynomial of F , and if one gets a non-zero remainder, then that remainder is added to the set so that eventually all elements of the new set have zero remainder after division. There is one more caveat — to make sense of polynomial division, we need to introduce an ordering to the monomials, and often it will simply be lexicographic ordering. And by division we mean, delete from the numerator the highest monomial that is a multiple of the leading monomial of the denominator by subtracting from the numerator the denominator with the appropriate proportionality term to cancel the said monomial.

Here's a simple example for the set of polynomials,

$$F = \{f_1, f_2\} = \{-27 + 18x^2 + 8x^3 + x^4 + 18y^2 - 24xy^2 + 2x^2y^2 + y^4, -4 + x^2 + y^2\}. \quad (1.26)$$

First, let's choose reverse lexicographic ordering so that $y > x$ and assign a set $G := F$, which is not yet the Gröbner basis. Buchberger tells us to cancel leading terms from all pairs in G , using the least common multiple of each leading term, and then divide the result through by the elements of G as much as possible. Since there are only two

polynomials, there is only one pair. By canceling the leading terms, shown in parenthesis, and then dividing through afterward (also called reducing), we get,

$$(f_1 - y^2 f_2) - x^2 f_2 + 24x f_2 - 22 f_2 = 61 - 96x + 32x^3, \quad (1.27)$$

which cannot be divided through anymore, so we define the remainder, $f_3 := 61 - 96x + 32x^3$, and add it to the set G . $(f_1 - y^2 f_2)$ now has zero remainder by construction. Now the next pair,

$$\begin{aligned} (32x^3 f_1 - y^4 f_3) - 96x f_1 + 61y^2 f_2 - 64x^5 f_2 + 768x^4 f_2 - 384x^3 f_2 - 2365x^2 f_2 \\ + 1728x f_2 + 244 f_2 + x^4 f_3 - 32x^3 f_3 - 8x^2 f_3 + 96x f_3 + 16 f_3 = 0, \end{aligned} \quad (1.28)$$

so there is no remainder. The next pair,

$$(32x^3 f_2 - y^2 f_3) - 96x f_2 + 61 f_2 - x^2 f_3 + 4 f_3 = 0, \quad (1.29)$$

also has no remainder. We've checked all pairs now, and each can be divided through with no remainder, and thus the set,

$$G = \{f_1, f_2, f_3\}, \quad (1.30)$$

is a Gröbner basis. Note that we've ended up with a larger set than we started with, and perhaps even worse it turns out that the Gröbner basis is not unique since you can just add any polynomial that has zero remainder to the set. There is a simple fix. If any basis element has a monomial which can be divided by the leading term of another basis element, then it can be reduced, and this process should be done and repeated until the leading terms cannot divide any monomial of any element of the set. The result is called the reduced Gröbner basis, and it is unique for a given monomial ordering. Note that most

software calculations output the reduced Gröbner basis. Continuing the example, from Eq. 1.27, shows that f_1 itself, (*i.e.*, without needing a least common multiple multiplier), can be divided (reduced) by f_2 and f_3 all the way to zero, so f_1 is unnecessary for the Gröbner basis. Thus, the reduced Gröbner basis is,

$$G = \{f_2, f_3\} = \{-4 + x^2 + y^2, 61 - 96x + 32x^3\}. \quad (1.31)$$

Notice what happened — the new term of our reduced Gröbner basis has eliminated the variable considered the highest by monomial ordering we chose — reverse lexicographical ordering. In this way, the Gröbner basis can be used to eliminate variables, and the variables to be eliminated should be assigned the greatest in the ordering, called the elimination order. See Fig. 1.9 for the two possible orderings, and the resulting Gröbner basis, from a software calculation.

```
In[1]:= {f1, f2} = {-27 + 18 x^2 + 8 x^3 + x^4 + 18 y^2 - 24 x y^2 + 2 x^2 y^2 + y^4, -4 + x^2 + y^2};
GroebnerBasis[{f1, f2}, {y, x}]
GroebnerBasis[{f1, f2}, {x, y}]

Out[2]= {61 - 96 x + 32 x^3, -4 + x^2 + y^2}

Out[3]= {-375 + 9216 y^2 - 6144 y^4 + 1024 y^6, 128 + 61 x - 160 y^2 + 32 y^4}
```

Figure 1.9: Gröbner basis calculations in Mathematica.

The Gröbner basis makes it easier to determine the solution to polynomial systems by eliminating variables. For completion, see Fig. 1.10 for the zeros of the two polynomials of F , where the above Gröbner basis gives a more direct route to the coordinates of the simultaneous zeros.

Finally, the last major tool that will be emphasized is the cylindrical decomposition [10]. In a nutshell, the cylindrical decomposition essentially solves systems of polynomial inequalities in $\mathbb{R}^d$ explicitly in terms of each variable, and is most sanely calculated via software implementation. Among its lengthy list of applications, it can be

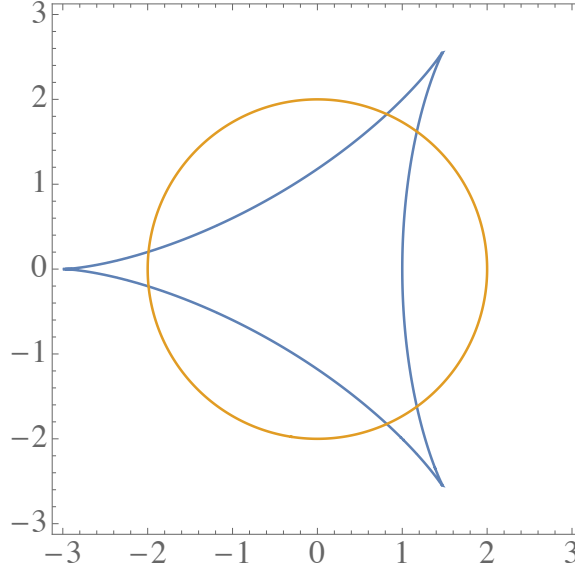


Figure 1.10: Intersecting algebraic curves of F from Eq. 1.26.

used to output machine generated proofs by eliminating quantifiers from formulas, and importantly for our purposes, it can find *projections* of semi-algebraic sets onto subspaces of $\mathbb{R}^d$.

A simple example will demonstrate how to find projections. Consider a Dupin cyclide defined as the solution set to,

$$(x^2 + y^2 + z^2)^2 - 4(5x - 12)^2 - 64y^2 < 0. \quad (1.32)$$

The cylindrical decomposition is given in Fig. 1.11.

To extract out the information about x and y only, that is, to project out only a certain variable, such as z , one can use quantifier elimination, see Fig. 1.12, where the existential quantifier is eliminated.

And see Fig. 1.13 for the Dupin cyclide volume, with its projections onto each coordinate plane easily obtained by the cylindrical decomposition algorithm.

Note that the cylindrical decomposition is not entirely unfamiliar, since it is used in basic calculus when integrating over volumes, volumes which need to be described in

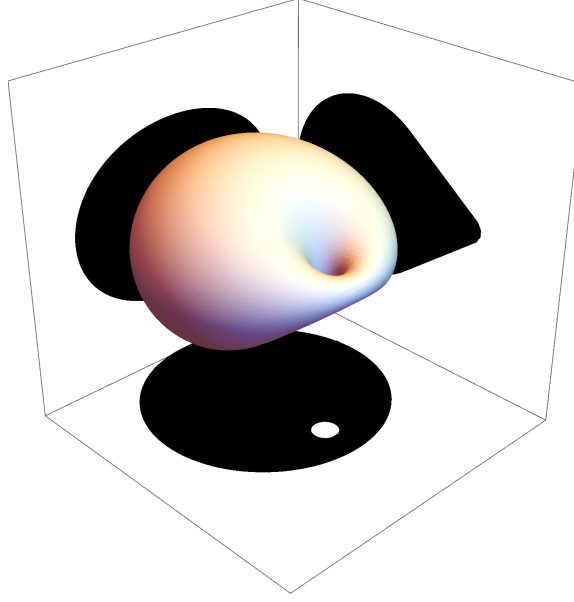


Figure 1.13: A Dupin cyclide and its coordinate plane projections.

1.3 Critical Points and Critical Values

A core element of this work is to describe semi-algebraic sets, which can be described by their boundaries. The following elementary notions have proven extremely useful when dealing with boundaries. The volume element of two spaces connected with a differentiable map, $(x_1, \dots, x_n) \mapsto (y_1, \dots, y_m)$ are related,

$$dy_1 \cdots dy_m = \sqrt{|\det g|} dx_1 \cdots dx_n, \quad (1.33)$$

where g is the induced metric with matrix elements $g_{ij} = \sum_k \frac{\partial y_k}{\partial x_i} \frac{\partial y_k}{\partial x_j}$. Note, that when $m = n$, the proportionality factor coincides with the Jacobian — in fact more generally, $\det g = \det(J^T J)$, where J is the rectangular Jacobian matrix. On the *boundary* of the image the volume element will vanish, so either $dx_i = 0$ for some i , or the metric becomes singular, meaning boundaries are mapped to boundaries or a singular metric determines the boundary. The points where the Jacobian matrix has a less than maximal rank, are called critical points. The image of critical points are called critical values. Sard's

theorem states that the critical values form a measure zero set, consistent in our case with boundaries being hypersurfaces whose coordinates satisfy polynomial equality constraints [11].

As usual, a basic example can illustrate the main points. Consider the map,

$$(x_1, x_2) \mapsto (y_1, y_2) = (x_1, x_1^2 + x_2^2), \quad (1.34)$$

with $x_1, x_2 \in [-1, 1]^2$. The Jacobian of the map is $J = \det \begin{pmatrix} 1 & 0 \\ 2x_1 & 2x_2 \end{pmatrix} = 2x_2$. One can easily compute the image of all the boundaries and the critical points to get the image of the entire map, see Fig. 1.14.

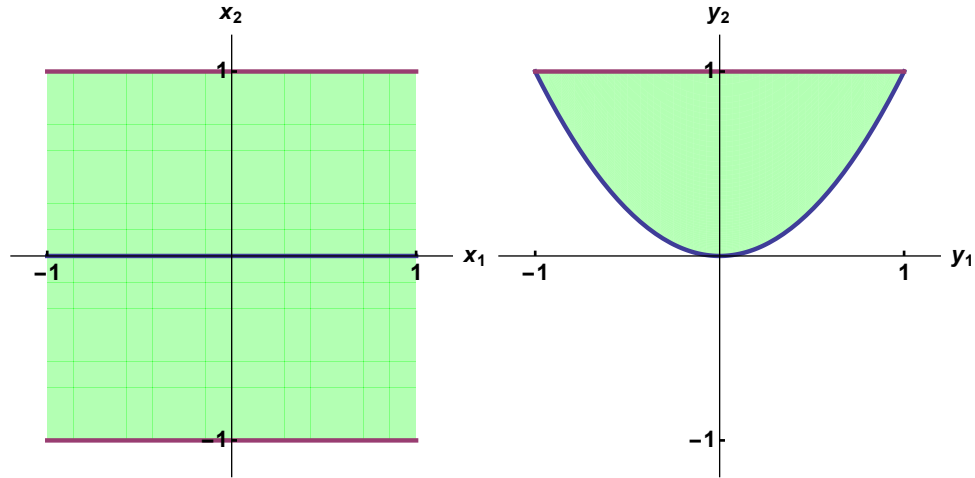


Figure 1.14: The boundaries in purple are mapped to boundaries in purple and critical points in blue are mapped to critical values in blue.

Chapter 2

The Tangle Constrained: Explorations with n -party States

The physical presence of entanglement permits access to and manipulation of various quantum mechanical information without the physical presence of each subsystem [12]. This remarkable privilege appears to come at a price however — as entanglement is found to be partner preferential, the postmodern polyamorist subculture is marginalized [13, 14, 15, 16, 17, 18], that is to say, the sharing of entanglement is limited by physical law. Therefore, a common milestone in quantum technology is sufficient control of substrates for the generation of highly multi-partite highly entangled states, for example, the Greenberger-Horne-Zeilinger state, $|\text{GHZ}\rangle = |0\rangle^{\otimes n} + |1\rangle^{\otimes n}$. This state alone has already garnered significant attention, providing stronger tests against local realism [19], improving precision atomic clocks [20] and interferometry [21] with possible implications for gravitational wave detection [22], thereby further motivating recipes for GHZ generation [23, 24, 25] with record setting confirmations in the qubit quantity on varying hardware [26, 27, 28, 29].

Once such a highly entangled state is obtained, the next cheapest layer of in-

formation processing consists of applying (stochastic) local operations and classical communications (SLOCC). Based on the presumed relative abundance of SLOCC implementation, the local operations serve another purpose — for the construction of a value to assign to states which lie outside SLOCC’s own ability to generate, *i.e.*, non-local states [30]. The value, as often the case, will simply be referred to as an amount of entanglement, ignoring potentially more fine-grained notions of the non-local resource.

Consider that if two states can be probabilistically transformed back *and* forth with SLOCC, the states should contain, in some sense, the same non-local resources, so that entanglement can be thought of as *invertible*-SLOCC invariant. In a SLOCC transformation, state norms only correspond to the success probability and are otherwise irrelevant, so it is convenient to identify invertible SLOCC operations with the classic unit determinant group $SL(2, \mathbb{C})^{\otimes n}$. It just so happens that any homogeneous SL invariant is guaranteed to be non-increasing on average under general quantum operations, and thus meets the standard prerequisite of entanglement monotonicity [31, 3, 32], also refer back to Chapter 1. As we will see, it is convenient and aesthetically pleasing to choose the generators of the algebra of SL invariants to be the relevant entanglement measures. The algebra of invariants for n copies of $SL(2, \mathbb{C})$ is partially known [33] and can be generated by the determinant for $n = 2$ [34], and the hyperdeterminant for $n = 3$ [35], which are often normalized to give the pure 2-tangle, $\tau_{A|B}(\psi_{i,j}) = 2|\det(\psi_{i,j})|$ and the pure 3-tangle, $\tau_{A|B|C}(\psi_{i,j,k}) = 2\sqrt{|\text{hdet}(\psi_{i,j,k})|}$ where ψ is the pure state tensor coefficients and the extra root on the 3-tangle ensures for both tangles identical transformation properties under local GL operations [36, 6]. Both tangles are extended to mixed states linearly on the particular pure state decomposition which provides the minimal average tangle, known as the convex roof [37, 38].

The celebrated results of Dür *et al.* [39] show that a generic 3-qubit pure state can be transformed to the GHZ state with SLOCC, meaning that a random sample from

Hilbert space will almost always produce a state connected to GHZ. By calculating tangles of the state $M_1 \otimes M_2 \otimes M_3 |\text{GHZ}\rangle$ with M_i any 2×2 complex matrix, which reaches almost all states, we derive a necessary and sufficient inequality to describe all possible *values* of tangles in three qubits, and we find this inequality to be strictly stronger than both monogamy [13] and marginal eigenvalue [40] inequalities. The crux of our results relies on the fact that the SLOCC invariants are *not* invariant when SLOCC acts externally to the relevant parties, in which case, we find the corresponding transformation rules simplify elegantly once restricted to the GHZ class; this chapter is about exploring the implications.

For more qubits, the GHZ class loses its generality, but we show that it retains a remarkable monogamy property as follows. Recall for arbitrary 3-qubit states, the total entanglement with any party A , $\tau_A = 2\sqrt{\det \rho_A}$, also known as the 1-tangle, decomposes exactly in terms of tangles with other parties B and C [13],

$$\tau_A^2 = \tau_{A|B}^2 + \tau_{A|C}^2 + \tau_{A|B|C}^2. \quad (2.1)$$

Recently, variations of the above have been conjectured to hold for all k -tangles in n -qubits, known as the strong monogamy relation [41] — the most natural generalization for n pure qubits is,

$$\tau_A^2 \stackrel{?}{=} \sum_{I_A} \tau_{I_A}^2, \quad (2.2)$$

where I_A is any subset of the n parties that includes the party A with $|I_A| \geq 2$. While strong monogamy *as such*, appears to be a stretch for arbitrary states [42], we find that it holds exactly on the GHZ SLOCC class. Thus we have excavated the very origin of the first law, Eq. 2.1, that effectively seeded the entire field of distributed entanglement theory. And finally, in salvation to the failure of Eq. 2.2 on all states, we describe a universal framework of entanglement constraints, in turn unearthing the origin of their

existence as well.

2.1 Three-Qubit Tangle Parametrization

Starting with three qubits, we calculate all of the tangles of the state, $M_1 \otimes M_2 \otimes M_3 |\text{GHZ}\rangle$. Mixed state 2-tangles have the following general formula, $\tau_{A|B}(\rho_{AB}) = \text{Max}(\sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}, 0)$, where the λ_i 's are the non-ascending eigenvalues of the operator $R = \rho_{AB}(\sigma_y \otimes \sigma_y) \rho_{AB}^T(\sigma_y \otimes \sigma_y)$ [37]. The 2-party marginals of the unnormalized $|\Psi_{ABC}\rangle = M_1 \otimes M_2 \otimes M_3 |\text{GHZ}\rangle$ are rank-2, and the 2-tangle can be quickly computed with the simplified formula,

$$\begin{aligned} p \tau_{A|B} &= \sqrt{\lambda_1} - \sqrt{\lambda_2} \\ &= \sqrt{\lambda_1 + \lambda_2 - 2\sqrt{\lambda_1 \lambda_2}} \\ &= \sqrt{\text{Tr}(R) - \sqrt{2(\text{Tr}(R)^2 - \text{Tr}(R^2))}}, \end{aligned} \quad (2.3)$$

with the now necessary explicit normalization factor $p = \langle \Psi_{ABC} | \Psi_{ABC} \rangle$. If we parametrize the M_i 's with two 2-component complex column vectors $M_i = (\underline{u}_i \ \underline{v}_i)$, where underscore means the coordinates of a geometric vector, then the resulting 2-tangle expression simplifies to $\tau_{A|B} = \frac{1}{p} |\vec{u}_1 \wedge \vec{v}_1| |\vec{u}_2 \wedge \vec{v}_2| |\vec{u}_3^\dagger \vec{v}_3|$, with $p = \frac{1}{2} |\vec{u}_1 \vec{u}_2 \vec{u}_3 + \vec{v}_1 \vec{v}_2 \vec{v}_3|^2$ and the vector juxtaposition means tensor product.

Due to the form of the expression with absolute values, complex numbers in the matrices M_i become redundant, and one can achieve the same values of the tangles with real matrices. Therefore it is convenient to parametrize the columns as $\underline{u}_i = (u_i \cos(\theta_i) \ u_i \sin(\theta_i))^T$ and $\underline{v}_i = (v_i \cos(\theta_i + \phi_i) \ v_i \sin(\theta_i + \phi_i))^T$, whence the tangle simplifies to $\tau_{A|B} = \frac{2}{p} u_1 u_2 u_3 v_1 v_2 v_3 |s_1 s_2 c_3|$, where $s_i = \sin \phi_i$ and $c_i = \cos \phi_i$, and $p = u_1^2 u_2^2 u_3^2 + v_1^2 v_2^2 v_3^2 + 2u_1 u_2 u_3 v_1 v_2 v_3 c_1 c_2 c_3$. Notice that the θ_i 's do not appear in

the expressions so we could set them to zero. Simplifying further, we get $\tau_{A|B} = |s_1 s_2 c_3| / (r + c_1 c_2 c_3)$, where $2r = u_1 u_2 u_3 / v_1 v_2 v_3 + v_1 v_2 v_3 / u_1 u_2 u_3$ and since all the $u_i, v_i \geq 0$, we have the bound $r \geq 1$ and consequentially, we only need to consider the case where $c_i \leq 0$. Accordingly, we shall make the minus sign on the c_i 's explicit and then only consider angles $\phi_i \in [0, \pi/2]$, which allows us to remove the absolute value signs. All of the 2-tangles can be cleansed of redundancy in an analogous manner, which then amounts to permuting the subscripts.

The 3-tangle can be calculated from the general formula [13],

$$\tau_{A|B|C}(\Psi) = \sqrt{2|\Psi_{j_5, j_4, j_3} \Psi_{j_2, j_1, j_0} \epsilon_{i_0, i_3} \epsilon_{j_0, j_3} \epsilon_{i_1, j_1} \epsilon_{i_2, j_2} \epsilon_{i_4, j_4} \epsilon_{i_5, j_5} \Psi_{i_5, i_4, i_3} \Psi_{i_2, i_1, i_0}|}, \quad (2.4)$$

with ϵ being the 2-index Levi-Civita symbol. It is easy to check that $\tau_{A|B|C}(|\text{GHZ}\rangle) = 1$, and then apply the transformation rule, $\tau(\otimes_p M_p |\text{GHZ}\rangle) = \prod_p |\det(M_p)| \tau(|\text{GHZ}\rangle) = \frac{1}{p} |\vec{u}_1 \wedge \vec{v}_1| |\vec{u}_2 \wedge \vec{v}_2| |\vec{u}_3 \wedge \vec{v}_3|$ with p as before. The result can then be reparametrized in the same manner as the 2-tangles; thus the tangle expressions only depend explicitly on four real parameters, $(r, \phi_1, \phi_2, \phi_3)$,

$$\begin{aligned} \tau_{B|C} &= \lambda c_1 s_2 s_3, & \tau_{A|C} &= \lambda s_1 c_2 s_3, \\ \tau_{A|B} &= \lambda s_1 s_2 c_3, & \tau_{A|B|C} &= \lambda s_1 s_2 s_3, \end{aligned} \quad (2.5)$$

where $c_i, s_i = (\cos)\sin(\phi_i)$, $\phi_i \in [0, \pi/2]$, $\lambda = 1/(r - c_1 c_2 c_3)$, and $r \geq 1$, noting the pleasing and perhaps surprising symmetry sparkling amongst the collection. This is a remarkable simplification because we have 4 different tangles and only 4 parameters. We can find constraints on the tangles by inverting the expressions, Eq. 2.5, using standard algebraic tools discussed in Chapter 1, leading to the following theorem.

2.2 Three-Party Achievability Theorem

Theorem: *Given an arbitrary 3-qubit pure state $|\Psi_{ABC}\rangle$, the corresponding tangles, $(\tau_{B|C}, \tau_{A|C}, \tau_{A|B}, \tau_{A|B|C}) \equiv (x, y, z, t)$, satisfy the following inequality,*

$$t^2(1 - x^2 - y^2 - z^2 - t^2) - (x^2y^2 + x^2z^2 + y^2z^2 - 2xyz) \geq 0. \quad (2.6)$$

Conversely, for any non-negative 4-tuple (x, y, z, t) satisfying the inequality, there exists a pure 3-qubit state with corresponding tangles.

To prove the theorem, it will be useful to invert the tangle expressions, Eq. 2.5, for the parameters. A Gröbner elimination based inversion must proceed in two calculations due to the degenerate case when $d = 2(r - c_1c_2c_3) = 0$. Therefore we set the single element Gröbner basis to zero, eliminating the angles, but keeping (x, y, z, t, d) ,

$$d(d^2(t^2 + x^2)(t^2 + y^2)(t^2 + z^2) - 4t^4) = 0. \quad (2.7)$$

We drop the degeneracy causing factor of $d = 0$, and add the remaining factor back to the same set of equations above. Computing another Gröbner basis for each variable, eliminating two angles each time as well as d , gives the following inversion,

$$c_1 = \frac{x}{\sqrt{t^2 + x^2}}, \quad c_2 = \frac{y}{\sqrt{t^2 + y^2}}, \quad c_3 = \frac{z}{\sqrt{t^2 + z^2}}, \quad (2.8)$$

which can then be back-substituted to find r as well,

$$r = \frac{t^2 + xyz}{\sqrt{(t^2 + x^2)(t^2 + y^2)(t^2 + z^2)}}. \quad (2.9)$$

The only non-trivial bound is $r \geq 1$, where by expanding the expression gives the inequality of the theorem, thus explicitly proving sufficiency.

To show necessity of the inequality, we just plug in expressions from Eq. 2.5 into the Eq. 2.6 and it can be simplified to,

$$\frac{s_1^2 s_2^2 s_3^2 (r^2 - 1)}{(r - c_1 c_2 c_3)^4} \geq 0, \quad (2.10)$$

and since $r \geq 1$, the inequality is true.

The above argument is only for *generic* states, and rather than appealing to continuity we'd like to provide additional proof that the inequality is true for *arbitrary* states. It will be convenient to use expressions for (x, y, z, t) from the 3-qubit Schmidt form [43, 44], using the unitary invariance of the invariants to simplify an arbitrary state,

$$\Psi = (a_1, a_2, a_3, a_4, a_5, a_6, a_7, a_8) \xrightarrow{U_A \otimes U_B \otimes U_C} (\lambda_0, 0, 0, 0, \lambda_1 e^{i\omega}, \lambda_2, \lambda_3, \lambda_4), \quad (2.11)$$

with real parameters $(\lambda_0, \lambda_1, \lambda_2, \lambda_3, \lambda_4, \omega) \geq 0$. The invariants can be computed straightforwardly *à la* Eq. 2.3,

$$x = 2|\lambda_2 \lambda_3 - e^{i\omega} \lambda_1 \lambda_4|, \quad y = 2\lambda_0 \lambda_2, \quad z = 2\lambda_0 \lambda_3, \quad t = 2\lambda_0 \lambda_4, \quad (2.12)$$

where again, $(\tau_{B|C}, \tau_{A|C}, \tau_{A|B}, \tau_{A|B|C}) \equiv (x, y, z, t)$. Notice that ω only varies x independently of the other invariants. The left-hand side of Eq 2.6, turns out to be concave in x , as seen by taking two derivatives,

$$\partial_x^2 [t^2(1 - x^2 - y^2 - z^2 - t^2) - (x^2 y^2 + x^2 z^2 + y^2 z^2 - 2xyz)] = -2(t^2 + y^2 + z^2), \quad (2.13)$$

so we only need to check for non-negativity with the extreme values of x , meaning $\omega = 0, \pi$. Plugging in expressions, Eq. 2.12 with the case of $\omega = \pi$, that is, $x = 2(\lambda_2 \lambda_3 + \lambda_1 \lambda_4)$,

turns the lhs of the inequality into,

$$(\lambda_0^2 + \lambda_1^2 + \lambda_2^2 + \lambda_3^2 + \lambda_4^2 - 1)g + [2\lambda_0(2\lambda_1\lambda_2\lambda_3 + \lambda_4 - 2\lambda_4(\lambda_2^2 + \lambda_3^2 + \lambda_4^2))]^2, \quad (2.14)$$

where g is some polynomial in the λ_i 's, but by applying normalization, $\lambda_0^2 + \lambda_1^2 + \lambda_2^2 + \lambda_3^2 + \lambda_4^2 = 1$, the first term vanishes regardless of the sign of g , and the remaining term is a perfect square, and hence non-negative certified. Now plugging in expressions for (x, y, z, t) in the other case of $\omega = 0$, that is, $x = 2(\lambda_2\lambda_3 - \lambda_1\lambda_4)$, assuming for now that $\lambda_2\lambda_3 \geq \lambda_1\lambda_4$, turns the lhs of the inequality into,

$$(\lambda_0^2 + \lambda_1^2 + \lambda_2^2 + \lambda_3^2 + \lambda_4^2 - 1)g' + [2\lambda_0(-2\lambda_1\lambda_2\lambda_3 + \lambda_4 - 2\lambda_4(\lambda_2^2 + \lambda_3^2 + \lambda_4^2))]^2, \quad (2.15)$$

with a new polynomial g' — amounting to a very minor change, but which importantly preserves the existence of a perfect square non-negative certificate. If we assume that $\lambda_2\lambda_3 \leq \lambda_1\lambda_4$, then the expressions of (x, y, z, t) , with $x = -2(\lambda_2\lambda_3 - \lambda_1\lambda_4)$, obviously satisfy,

$$t^2(1 - x^2 - y^2 - z^2 - t^2) - (x^2y^2 + x^2z^2 + y^2z^2 + 2xyz) \geq 0, \quad (2.16)$$

where the only change from the theorem's inequality is a minus sign on the x with a unit exponent. The above constraint is actually a stronger constraint than the theorem's inequality and therefore the theorem is proved.

See Fig. 2.1 for the solution set of Eq. 2.6, over the extended region, $[-1, 1]^3$ in the (x, y, z) -subspace, for various values of $t^2 \in [-1, 1]$; the black straight lines form the wire frame of the tetrahedral envelope. Note that an imaginary value for the 3-tangle is clearly non-sensical, however we soon find that corresponding surfaces are physically relevant.

With the above achievable set of tangles being described by a single inequality, it

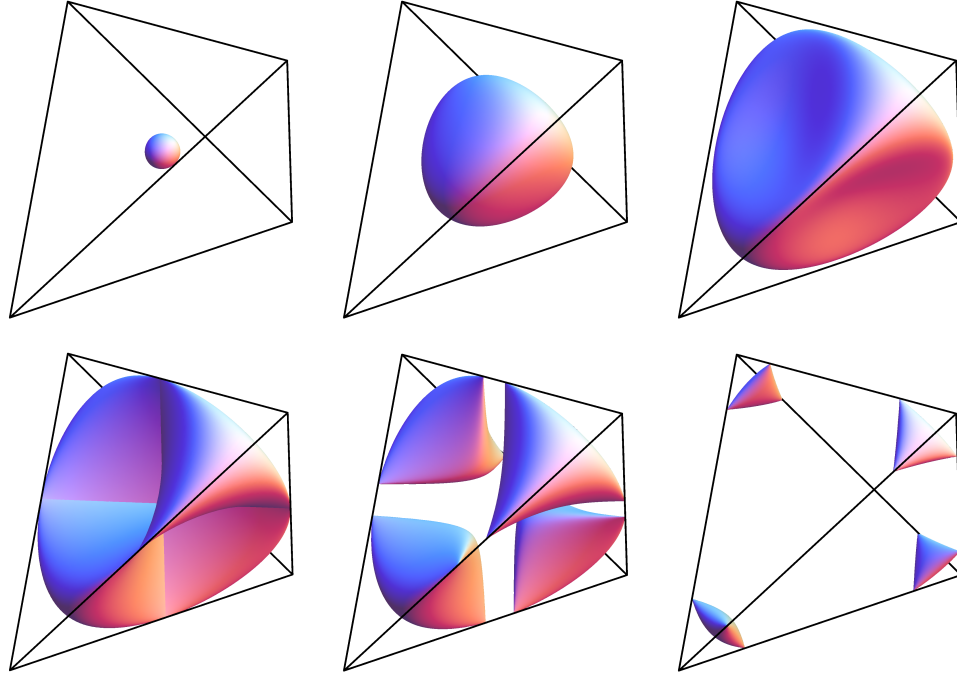


Figure 2.1: Envelope of slices to solution set of Eq. 2.6 for $t^2 = (.98, .64, .09, 0, -.01, -.25)$.

is straightforward to project out the 3-tangle, *i.e.*, take the union of $0 \leq t \leq 1$ slices, and get a constraint on 2-tangles alone, as similarly discussed in Chapter 1. It turns out this set can also be described by a single inequality. By noticing that Eq. 2.6 is quadratic in t^2 , we complete the square,

$$(1 - 2t^2 - x^2 - y^2 - z^2)^2 \leq (1 + x + y + z)(1 + x - y - z)(1 - x + y - z)(1 - x - y + z), \quad (2.17)$$

and we take the root, setting $t = 0$ to unconstrain (x, y, z) as much as possible, which gives the necessary and sufficient 2-tangle achievability inequality, reproducing the results of [45], and summarized further below.

It is often glossed over that the 2-tangles are defined as the minimum over all possible averages in a mixed state (the convex roof construction). The maximum average

can also reveal useful information. Known through the *concave* roof construction [4] (as in Chapter 1), the maximum average tangle in mixed states is commonly referred to as the tangle of assistance. The 2-tangle of assistance is not an entanglement monotone on 2-qubit states, however, it is an entanglement monotone on 3-qubits when evaluated among any 2-qubit pair [46] and may be related in a simple way to violations of Mermin inequalities [47]. Since the tangle of assistance gives information about 3-qubit entanglement, one expects it to be related to the 3-tangle. Indeed, the following relation holds for any 3-qubit pure state, $|\Psi_{ABC}\rangle$:

$$\tau_{A|B|C}^2 = \hat{\tau}_{A|B}^2 - \check{\tau}_{A|B}^2 = \hat{\tau}_{A|C}^2 - \check{\tau}_{A|C}^2 = \hat{\tau}_{B|C}^2 - \check{\tau}_{B|C}^2, \quad (2.18)$$

where $\hat{\tau}$ denotes the concave roof tangle, and $\check{\tau}$ denotes the convex roof tangle (being the same tangle from the theorem), so that the 3-tangle is the difference between the maximal and minimal 2-tangle among any pair. When the above is rearranged and substituted into Eq. 2.6, one gets a necessary and sufficient 2-tangle of assistance inequality, however, peculiarly, if we examine the boundary, by turning the inequality into an equality, and squaring away the square root that appears, then factoring the result, we get the following polynomial as a factor,

$$-t^2(1 - x^2 - y^2 - z^2 + t^2) - (x^2y^2 + x^2z^2 + y^2z^2 - 2xyz) = 0, \quad (2.19)$$

where now $(\hat{\tau}_{A|B}, \hat{\tau}_{A|C}, \hat{\tau}_{B|C}, \tau_{ABC}) \equiv (x, y, z, t)$. Note the curious relation to Eq. 2.6 by a Wick-like rotation, $t \rightarrow it$. Revisit Fig. 2.1 for the solution set of Eq. 2.6 for various values of $t^2 \in [-1, 1]$. One can take the union of imaginary t slices by a similar method as the real t slices, which we summarize in the following theorem which includes both convex and concave roof cases distinguished with parenthesis and the symbol $\pm$ respectively.

Corollary: *Given an arbitrary 3-qubit pure state $|\Psi_{ABC}\rangle$, its pairwise convex*

(concave) roof 2-tangles, $(\tau_{A|B}, \tau_{A|C}, \tau_{B|C}) \equiv (x, y, z)$, satisfy the following inequality,

$$\sqrt{(1-x-y+z)(1-x+y-z)(1+x-y-z)(1+x+y-z)} \pm (1-x^2-y^2-z^2) \geq 0. \quad (2.20)$$

Conversely, for any non-negative triple (x, y, z) satisfying the inequality, there exists a pure 3-qubit state with corresponding convex (concave) roof 2-tangles.

The solution set of the inequalities are variations on the famous Roman Steiner surface, see Fig. 2.2 where the parenthesis again indicates separate cases.

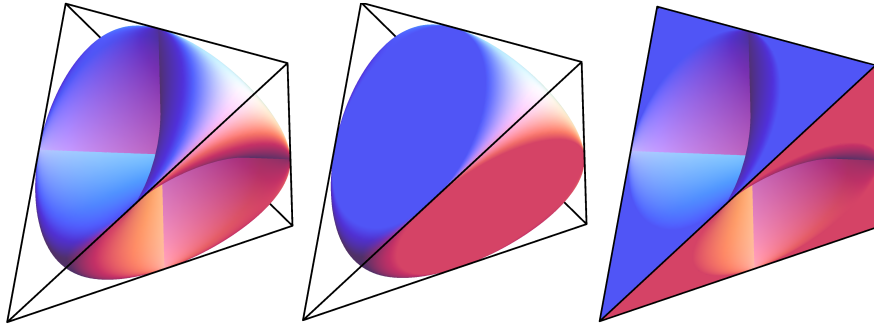


Figure 2.2: The Steiner Suite. Achievable 2-tangles (of assistance) form the non-negative component of the Steiner surface's (inverted) convex hull. The Steiner volume on the left can be thought of as coming from states in the null cone $\tau_{A|B|C} = 0$ whose mixed 2-tangles are independent of the decomposition $\hat{\tau}_{i|j} = \check{\tau}_{i|j}$.

The convex hull of the surface has also shown up in a number of places, *e.g.*, the parametrization of tripartite Werner states where 2-party marginals are constrained to be local-positive [48], in the image set of a triple of hermitian matrices [49], and finally in a quite peculiar classical/quantum duality [50, 45, 51].

2.3 Marginal Eigenvalues and 1-tangles

The story so far is similar in spirit to the marginal problem — given subsystem information, what are the consistency conditions for a joint state? Recall Eq. 2.1, and

that the 1-tangle can be written in terms of the minimal single party eigenvalue, λ_A , $\tau_A = 2\sqrt{\lambda_A(1-\lambda_A)}$, so we can relate the eigenvalues and invariants,

$$\lambda_A = \frac{1}{2} \left(1 - \sqrt{1 - \tau_{A|B}^2 - \tau_{A|C}^2 - \tau_{A|B|C}^2} \right). \quad (2.21)$$

where other relations are obtained by permuting the parties and each λ_P is the smallest eigenvalue of party P . Inverting, we get,

$$\tau_{A|B} = \sqrt{2\lambda_A(1-\lambda_A) + 2\lambda_B(1-\lambda_B) - 2\lambda_C(1-\lambda_C) - \tau_{A|B|C}^2/2}, \quad (2.22)$$

where again, other relations are obtained by permuting the parties. We substitute into the inequality of theorem to get the following,

$$\begin{aligned} & \tau_{A|B|C}^2 - \tau_{A|B|C}^4/4 + 4(\lambda_A^4 + \lambda_B^4 + \lambda_C^4) - 8(\lambda_A^3 + \lambda_B^3 + \lambda_C^3) + 4(\lambda_A^2 + \lambda_B^2 + \lambda_C^2) \\ & + 8(\lambda_A(1-\lambda_A)\lambda_B(1-\lambda_B) + \lambda_A(1-\lambda_A)\lambda_C(1-\lambda_C) + \lambda_B(1-\lambda_B)\lambda_C(1-\lambda_C)) \\ & + 2\sqrt{2\lambda_A(1-\lambda_A) + 2\lambda_B(1-\lambda_B) - 2\lambda_C(1-\lambda_C) - \tau_{A|B|C}^2/2} \\ & \times \sqrt{2\lambda_A(1-\lambda_A) - 2\lambda_B(1-\lambda_B) + 2\lambda_C(1-\lambda_C) - \tau_{A|B|C}^2/2} \\ & \times \sqrt{-2\lambda_A(1-\lambda_A) + 2\lambda_B(1-\lambda_B) + 2\lambda_C(1-\lambda_C) - \tau_{A|B|C}^2/2} \geq 0. \end{aligned} \quad (2.23)$$

The 3-tangle can be projected out to recover the marginal eigenvalue inequality. Since it is easier to work with polynomials, we will take the above inequality, turn it into an equality and square away the root. The resulting expression has two factors, $p_1 p_2 = 0$,

where,

$$\begin{aligned}
p_1 &= \tau_{A|B|C}^4 + 16(1 + \lambda_A - \lambda_B - \lambda_C)(1 - \lambda_A + \lambda_B - \lambda_C) \\
&\quad \times (1 - \lambda_A - \lambda_B + \lambda_C)(1 - \lambda_A - \lambda_B - \lambda_C), \\
p_2 &= \tau_{A|B|C}^4 + 16(\lambda_A - \lambda_B - \lambda_C)(-\lambda_A + \lambda_B - \lambda_C)(-\lambda_A - \lambda_C + \lambda_C)(2 - \lambda_A - \lambda_B - \lambda_C).
\end{aligned} \tag{2.24}$$

Each factor can be thought of as the boundary of the maximal eigenvalues, or the minimal eigenvalues of each party since the factors are related by a substitution, $\lambda_P \mapsto 1 - \lambda_P$. Of the two factors, the latter will determine the constraint on the minimal eigenvalues. One can again simply set $\tau_{A|B|C} = 0$, to maximally unconstrain the eigenvalues, and it is then valid to drop the last factor, $(2 - \lambda_A - \lambda_B - \lambda_C)$, since it has no bearing on the minimal eigenvalues due to $\lambda_P \leq 1/2$. Thus we recover the marginal eigenvalue bound,

$$(\lambda_A - \lambda_B - \lambda_C)(-\lambda_A + \lambda_B - \lambda_C)(-\lambda_A - \lambda_B + \lambda_C) \geq 0, \tag{2.25}$$

It is worth pointing out that one can rewrite this expression back in terms of the 1-tangles with the substitution, $\lambda_i = \frac{1}{2}(1 - \sqrt{1 - \tau_i^2})$ and further, the above marginal inequality has been extended to arbitrary numbers of pure qubits [40], so the distribution of 1-tangles is hence likewise a fully solved problem. See Fig. 2.3 to see what the set of triples (τ_A, τ_B, τ_C) looks like in 3-qubits.

2.4 Parametrization of k -tangles and Strong Monogamy

So far everything discussed follows readily from the tangle expressions of Eq. 2.5, yet the obvious symmetry still seems to be begging to be let further out of the box — let us preemptively generalize to arbitrary numbers of qubits for our main result, writing

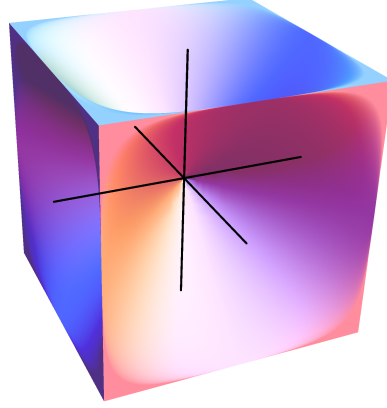


Figure 2.3: Achievable 1-tangles in 3-qubits form the non-negative component of the pictured volume. Note, the faces of the cube have been bored to the origin.

down the expressions for the tangles, and afterwards discuss how we can derive the expressions in two independent ways.

Proposition: *Let $\mathcal{P}$ be a set of n parties. The k -tangle between a subset of parties $I \subseteq \mathcal{P}$ with $|I| = k \geq 2$, of the n -qubit state, $|\psi\rangle = \otimes_{p \in \mathcal{P}} M_p |\text{GHZ}\rangle$, is given by,*

$$\tau_I = \frac{1}{r - \prod_{p \in \mathcal{P}} c_p} \prod_{i \in I} s_i \prod_{\bar{i} \in \bar{I}} c_{\bar{i}}, \quad (2.26)$$

and the 1-tangle, for any single party A , is given by,

$$\tau_A = \frac{1}{r - \prod_{p \in \mathcal{P}} c_p} s_A \sqrt{1 - \prod_{i \in \mathcal{P} \setminus \{A\}} c_i^2}, \quad (2.27)$$

where each $M_p \in \mathbb{C}^{2 \times 2}$, and without loss of generality, we choose a non-redundant real parametrization $M_p = \begin{pmatrix} u_p & v_p c_p \\ 0 & v_p s_p \end{pmatrix}$ with $u_p, v_p \geq 0$ and $c_p, s_p = (\cos) \sin(\phi_p)$ and $2r = \prod_{p \in \mathcal{P}} \frac{u_p}{v_p} + \prod_{p \in \mathcal{P}} \frac{v_p}{u_p}$.

Note that Eq. 2.2 is satisfied by these tangles, which follows from a trivial trigonometric identity, $\prod_k (s_k^2 + c_k^2) = 1$. Therefore, this is the first family of states that satisfy the strong monogamy equality with all k -tangles supported [52].

We now justify our formula for the k -tangle in two ways, each of which stems from equally acceptable interpretations of Eq. 2.1. One can equally think of Eq. 2.1 as the definition of the 3-tangle as the residual entanglement — that which is left over from the 1-tangle and its natural decomposition into pairwise 2-tangles. One can continue to recursively define the residual entanglement for a set of $\mathcal{P}$ qubits, defined on pure states as $\tau_{\text{res}} = \tau_{\mathcal{P}} = \sqrt{\tau_A^2 - \sum_{I_A \subset \mathcal{P}} \tau_{I_A}^2}$ and extended to mixed states *via* convex roof, and it is this interpretation of the k -tangle which was used in the first suggestions of strong monogamy [41].

For our proposition, first define $|\text{GHZ}\rangle_{a,b} = a|0\rangle^{\otimes n} + b|1\rangle^{\otimes n}$, and since a loss of any qubit results in a separable state, we have $\tau_{\text{res}}(|\text{GHZ}\rangle_{a,b}) = \tau_A(|\text{GHZ}\rangle_{a,b}) = 2|ab|$ for any party A . Notice the *same* formula results from the 2-tangles on the same pure 2-qubit GHZ state. We can therefore use the 2-tangle mixed state formula to compute the residual tangle on a mixture of two n -qubit $|\text{GHZ}\rangle_{a,b}$ states with differing a, b , since *every* corresponding pure state decomposition will be a mixture of only GHZ states (where the minimum is already known by the 2-tangle formula). A mixture of two GHZ states forms a matrix which has its only non-zero block on the $|0\rangle^{\otimes n}, |1\rangle^{\otimes n}$ subspace — the tangle computation gives, $\tau_{\text{res}} \begin{pmatrix} \alpha & \beta \\ \bar{\beta} & \gamma \end{pmatrix} = 2|\beta|$. The result can be applied to the following subsystem, for general $M_p = (\underline{u}_p, \underline{v}_p), \vec{u}_p, \vec{v}_p \in \mathbb{C}^{\otimes 2}$,

$$\begin{aligned} \rho_I &= \text{Tr}_{\bar{I}}(\otimes_{\bar{i} \in \bar{I}} M_{\bar{i}} |\text{GHZ}\rangle) \\ &= \begin{pmatrix} \prod_{\bar{i}} \vec{u}_{\bar{i}}^\dagger \vec{u}_{\bar{i}} & \prod_{\bar{i}} \vec{u}_{\bar{i}}^\dagger \vec{v}_{\bar{i}} \\ \prod_{\bar{i}} \vec{v}_{\bar{i}}^\dagger \vec{u}_{\bar{i}} & \prod_{\bar{i}} \vec{v}_{\bar{i}}^\dagger \vec{v}_{\bar{i}} \end{pmatrix}, \end{aligned} \quad (2.28)$$

where what is shown is the only non-zero block which has its support in the $|0\rangle^{\otimes n}, |1\rangle^{\otimes n}$ subspace. Notice that the $M_{\bar{i}}$'s here are acting externally to I . These residual tangles can be shown inductively to transform under internal SLOCC on the pure GHZ class

as $\tau_{\text{res}}(\otimes_k M_k | \text{GHZ}) = \prod_k |\det(M_k)| \tau_{\text{res}}(| \text{GHZ} \rangle)$, and if the rule holds on pure states, it also holds on mixed states. The base case of the 2-tangles is already known to obey the transformation rules on pure and mixed states. Assuming the transformation rules hold for the k -tangles, $k < n$, we can assume the validity of expressions in the proposition (except the n -tangle), but Eq. 2.2 then defines the n -tangle, which thus gives the formula in the proposition as well as the transformation rule on pure states. The extension of the transformation rule to mixed states is a result of Tajima [6]. So as long as an M_i isn't traced over, it can be factored out of the tangle as a determinant. Thus when all is fully evaluated, we reproduce the tangle expressions from the proposition.

The previous interpretation of k -tangles as residual tangles has the sense of a tautology, since Eq. 2.2 is, after all, the definition of the n -qubit n -tangle as a residual tangle. Just as in the 3-qubit case, there is an independent interpretation of k -tangles which arrives at the same, Eq. 2.2, in a highly non-obvious way — as a coincidence from taking the 3-tangle defined as an SL invariant. Depending on the parity of the number of qubits, we write the k -tangle as the magnitude of an anti-linear operator's expectation value. For even number of pure qubits, define $\tau_{\mathcal{P}} = |\langle \Psi^* | \Theta^{(+)} | \Psi \rangle|$, with matrix elements $\Theta_{i,j}^{(+)} = \prod_{l=0}^{k-1} \epsilon_{i_l, j_l}$ where i_l is the l th bit of the binary expansion of i , $|\mathcal{P}| = k$, and ϵ is the 2-index Levi-Civita symbol, and this k -tangle is sometimes known as Caley's *other* hyperdeterminant, and has been considered by several others [53, 54, 55, 33]. Due to the anti-linear hermiticity, a complete formula for the convex roof is given in [4] as a generalization of Woottter's formula,

$$\tau_I(\rho_I) = \text{Max}(\sqrt{\lambda_1} - \sum_{i \geq 2} \sqrt{\lambda_i}, 0), \quad (2.29)$$

with λ_i 's the non-ascending eigenvalues of $R = \rho_I \Theta^{(+)} \rho_I \Theta^{(+)}$. The tangle transforms as usual under internal local GL operations, and a direct calculation with Eq 2.28 and

Eq. 2.3 readily recovers the expressions in the proposition.

For odd number of qubits, $|\langle \Psi^* | \Theta^{(+)} | \Psi \rangle| = 0$ on all states and we actually must use at least a degree-4 invariant [33]. In that case, we will write the tangle as an expectation value of an operator with the state embedded into a space of squared size, $\sqrt{2} |\langle \Psi^* | \langle \Psi^* | \Theta^{(-)} | \Psi \rangle | \Psi \rangle|$, where the matrix elements are given as,

$$\Theta_{i,j}^{(-)} = \epsilon_{i_0,i_k} \epsilon_{j_0,j_k} \prod_{l=1}^{k-1} \epsilon_{i_l,j_l} \epsilon_{i_{k+l},j_{k+l}}, \quad (2.30)$$

which again has an analogous formula for the convex roof [4]. There is an ambiguity in how to embed an odd k -qubit mixed state into $2k$ -qubit space, we propose the option, $\rho \mapsto \rho \otimes \rho$. With this definition of the odd k -tangle, the formulas in the proposition can be reproduced.

The above two interpretations of the k -tangle are not expected to be the same in general, so it is further surprising that they agree at all on the GHZ class.

2.5 A Notable Property of the k -tangle

It is worth pointing out that these k -tangles generalize other properties of the 2- and 3-tangle, for example for arbitrary I odd qubits,

$$\tau_I = \hat{\tau}_{I \setminus \{A\}}^2 - \check{\tau}_{I \setminus \{A\}}^2, \quad (2.31)$$

generalizing Eq. 2.18, recycling the notation of hat for concave roof and check for convex roof, and we prove the relation with a direct calculation. Consider the definition,

$$\begin{aligned} \tau_I^2 &= 2 |\langle \Psi^* | \langle \Psi^* | \Theta^{(-)} | \Psi \rangle | \Psi \rangle| \\ &= 2 \sqrt{\langle \Psi^* | \langle \Psi^* | \Theta^{(-)} | \Psi \rangle | \Psi \rangle \langle \Psi | \langle \Psi | \Theta^{(-)} | \Psi^* \rangle | \Psi^* \rangle}, \end{aligned} \quad (2.32)$$

and write out the term under the root in components as,

$$\Psi_{i_0, i_<} \Psi_{i_k, i_>} \Psi_{j_0, j_<} \Psi_{j_k, j_>} \Psi_{a_0, a_<}^* \Psi_{a_k, a_>}^* \Psi_{b_0, b_<}^* \Psi_{b_k, b_>}^* \epsilon_{i_0, i_k} \epsilon_{j_0, j_k} \epsilon_{a_0, a_k} \epsilon_{b_0, b_k} \epsilon_{i, j}^{<} \epsilon_{i, j}^{>} \epsilon_{a, b}^{<} \epsilon_{a, b}^{>}, \quad (2.33)$$

where we use compact notation to save space, $i_< = i_1, \dots, i_{k-1}$, $i_> = i_{k+1}, \dots, i_{2k-1}$ and $\epsilon_{i, j}^{<} = \prod_{l=1}^{k-1} \epsilon_{i_l, j_l}$, $\epsilon_{i, j}^{>} = \prod_{l=1}^{k-1} \epsilon_{i_{k+l}, j_{k+l}}$. Note, we have specifically shunned the 0-bit and k -bit indices from the compacted notation for isolated computations. By applying the identity, $\epsilon_{i, i'} \epsilon_{j, j'} = \delta_{i, j} \delta_{i', j'} - \delta_{i, j'} \delta_{i', j}$, between i 's and a 's, and again between j 's and b 's, we get,

$$\begin{aligned} \epsilon_{i_0, i_k} \epsilon_{j_0, j_k} \epsilon_{a_0, a_k} \epsilon_{b_0, b_k} &= (\delta_{i_0, a_0} \delta_{i_k, a_k} - \delta_{i_0, a_k} \delta_{i_k, a_0}) (\delta_{j_0, b_0} \delta_{j_k, b_k} - \delta_{j_0, b_k} \delta_{j_k, b_0}) \\ &= \delta_{i_0, a_0} \delta_{i_k, a_k} \delta_{j_0, b_0} \delta_{j_k, b_k} - \delta_{i_0, a_0} \delta_{i_k, a_k} \delta_{j_0, b_k} \delta_{j_k, b_0} \\ &\quad - \delta_{i_0, a_k} \delta_{i_k, a_0} \delta_{j_0, b_0} \delta_{j_k, b_k} + \delta_{i_0, a_k} \delta_{i_k, a_0} \delta_{j_0, b_k} \delta_{j_k, b_0}. \end{aligned} \quad (2.34)$$

Now, we simplify each term, one at a time within Eq. 2.33. The first term gives,

$$\begin{aligned} &\Psi_{i_0, i_<} \Psi_{i_k, i_>} \Psi_{j_0, j_<} \Psi_{j_k, j_>} \Psi_{a_0, a_<}^* \Psi_{a_k, a_>}^* \Psi_{b_0, b_<}^* \Psi_{b_k, b_>}^* \delta_{i_0, a_0} \delta_{i_k, a_k} \delta_{j_0, b_0} \delta_{j_k, b_k} \epsilon_{i, j}^{<} \epsilon_{i, j}^{>} \epsilon_{a, b}^{<} \epsilon_{a, b}^{>} \\ &= \rho_{i_<, a_<} \rho_{i_>, a_>} \rho_{j_<, b_<} \rho_{j_>, b_>} \epsilon_{i, j}^{<} \epsilon_{i, j}^{>} \epsilon_{a, b}^{<} \epsilon_{a, b}^{>} \\ &= (\rho_{i_<, a_<} \epsilon_{a, b}^{<} \rho_{b_<, j_<}^T \epsilon_{j, i}^{<}) (\rho_{i_>, a_>} \epsilon_{a, b}^{>} \rho_{b_>, j_>}^T \epsilon_{j, i}^{>}) \\ &= \text{Tr}(R)^2, \end{aligned} \quad (2.35)$$

with $\rho_{i_<,a_<} = \Psi_{i_0,i_<} \Psi_{a_0,a_<}^* \delta_{i_0,a_0}$ being the components of $\rho_{I \setminus \{A\}} = \text{Tr}_A |\Psi_I\rangle \langle \Psi_I|$, and $R = \rho_{I \setminus \{A\}} \Theta^{(+)} \rho_{I \setminus \{A\}}^T \Theta^{(+)}$. The second term gives,

$$\begin{aligned}
& \Psi_{i_0,i_<} \Psi_{i_k,i_>} \Psi_{j_0,j_<} \Psi_{j_k,j_>} \Psi_{a_0,a_<}^* \Psi_{a_k,a_>}^* \Psi_{b_0,b_<}^* \Psi_{b_k,b_>}^* \delta_{i_0,a_0} \delta_{i_k,a_k} \delta_{j_0,b_0} \delta_{j_k,b_0} \epsilon_{i,j}^{<} \epsilon_{i,j}^{>} \epsilon_{a,b}^{<} \epsilon_{a,b}^{>} \\
&= \rho_{i_<,a_<} \rho_{i_>,a_>} \rho_{j_<,b_<} \rho_{j_>,b_>} \epsilon_{i,j}^{<} \epsilon_{i,j}^{>} \epsilon_{a,b}^{<} \epsilon_{a,b}^{>} \\
&= (\rho_{i_<,a_<} \epsilon_{a,b}^{<} \rho_{b_<,j_>}^T \epsilon_{j,i}^{>}) (\rho_{i_>,a_>} \epsilon_{a,b}^{>} \rho_{b_>,j_<}^T \epsilon_{j,i}^{<}) \\
&= \text{Tr}(R^2),
\end{aligned} \tag{2.36}$$

using the same notation as before. The third and fourth term calculations recapitulate the first and second, and therefore we have the following,

$$\begin{aligned}
\tau_I^2 &= 2\sqrt{2(\text{Tr}(R)^2 - \text{Tr}(R^2))} \\
&= \text{Tr}(R) + \sqrt{2(\text{Tr}(R)^2 - \text{Tr}(R^2))} \\
&\quad - \left(\text{Tr}(R) - \sqrt{2(\text{Tr}(R)^2 - \text{Tr}(R^2))} \right) \\
&= (\sqrt{\lambda_1} + \sqrt{\lambda_2})^2 - (\sqrt{\lambda_1} - \sqrt{\lambda_2})^2 \\
&= \hat{\tau}_{I \setminus \{A\}}^2 - \check{\tau}_{I \setminus \{A\}}^2,
\end{aligned} \tag{2.37}$$

so that these generalized k -tangles maintain similar properties of the few-party tangles as one might expect, recall Eq 2.3 and Eq 2.18.

2.6 All Polynomial Invariants are Constrained

Since strong monogamy is known to not hold in general [42], it is quite curious that Eq. 2.2 holds at all. The equation is a relation among low degree polynomial invariants, so we suppose that this special property may be a consequence of algebraically independent high degree invariants vanishing on the GHZ state. Such a guess is supported in four qubits, as the fundamental SL invariants evaluate on the GHZ state as

$(H^{(2)}, M^{(4)}, L^{(4)}, D_{xt}^{(6)}) = (1, 0, 0, 0)$, using the notation in [53], with the degrees written in the exponents.

Rather than try to rehabilitate the globally broken strong monogamy, let us paint a different picture. The take-home lesson that monogamy taught us is that the tensor product structure limits the way in which a multipartite wave function can be compatible with the tensor factors of Hilbert space. Compatibility can be well-captured by inequalities on polynomial entanglement measures. Consider a space whose dimensions are placeholders for state coefficients of a multipartite wavefunction (thought of as a real space of twice the dimension) in addition to some number of polynomial entanglement invariants, $\{(\psi_i, I_j)\}$. An algebraic variety is defined within this space by the relationships between the invariants and the state coefficients $\{(\psi_i, I_j) | f_k(\psi_i, I_j) = 0\}$, where the f 's are algebraic functions. We can project out all of the state variables from the variety to get exact constraints on the allowed entanglement invariants. Invoking the Tarski-Seidenberg theorem [10], which states the projection of a semi-algebraic set is again a semi-algebraic set, then proves that the achievable set of any collection of polynomial entanglement measures (a projection) is described by a collection of semi-algebraic relations on those measures. The advantage of this framework is that the resulting inequalities are not only necessary, but also sufficient.

One algorithm in particular is known for performing such projections, the cylindrical decomposition (as mentioned in Chapter 1), however it is in general a doubly exponential algorithm in the number of dimensions [10]. The 3-qubit case is the simplest system where non-trivial entanglement trade-off appears, yet it seems inefficient for the algorithm to handle blindly. Therefore, we have simplified the problem, to, in a sense, manually perform the projection. We have then given a few concrete examples of the Tarski-Seidenberg theorem in action (some other examples can be found in [56, 45, 51]) which in our case has led us to even stronger constraints beyond monogamy. Inasmuch

as the GHZ state is an economically viable reagent in quantum experimentation and can provide an operational meaning to the k -tangle, a comprehensible theory of multi-partite entanglement may be a step closer to being within grasp. On the other hand, it is known that the marginal inequalities become drastically complicated [57], while still remaining linear in eigenvalues, and we thus might expect semi-algebraic relations on invariants, which apparently imply marginal constraints, to become even more vastly complicated.

2.7 Miscellaneous Weak Monogamy

In the above, we found states which achieve equality in the strong monogamy inequality. Here we give states which achieve equality in weaker monogamy relations. First, the very original 2-tangle monogamy inequality,

$$\tau_A^2 \geq \sum_{|I_A|=2} \tau_{I_A}^2, \quad (2.38)$$

where only 2-tangles with party A appear on the right hand side, is a necessary condition for all n -qubit states [14], and states which achieve equality are the following,

$$|W\rangle = w_1 |0 \dots 01\rangle + w_2 |0 \dots 10\rangle + \dots + w_n |10 \dots 00\rangle, \quad (2.39)$$

where only Hamming weight one states appear, and is known as the W -family, and that they achieve monogamy equality has been known from the beginning [13]. In the case of this weaker monogamy relation, we can go a little further and show *sufficiency*. We will start with the W family (on the boundary) and add a few more parameters to fill the

space. Consider the following states,

$$|\Psi\rangle = c|0\rangle + \sum_{j=1}^n w_j |2^{j-1}\rangle + \sum_{0 < k \neq 2^\ell}^{2^{n-1}} b_k |k\rangle. \quad (2.40)$$

As a column matrix, exactly $2^{n-1} - 1$ of the components are zero, the w 's correspond to hamming weight one states, and the b 's fill out the rest. For simplicity, let $w, b, c \geq 0$ be real. We find the reduced density matrices,

$$\begin{aligned} \rho_{n,\eta} &= \text{Tr}_{\hat{n}, n-1, \dots, \hat{\eta}, \dots, 1} |\Psi\rangle \langle \Psi| \\ &= \begin{pmatrix} \rho_{00} & \rho_{01} & cw_n & 0 \\ \rho_{01} & w_\eta^2 + \sum_{(k_\eta=1)} b_k^2 & w_\eta w_n & 0 \\ cw_n & w_\eta w_n & w_n^2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \end{aligned} \quad (2.41)$$

where we leave ρ_{00}, ρ_{01} unspecified since the result is independent of their value, and k_η means the η th bit of the binary expansion of k . Direct calculation shows that $R = \rho_{n,\eta}(\sigma_y \otimes \sigma_y) \rho_{n,\eta}^T(\sigma_y \otimes \sigma_y)$ has a rank of two, and we use the rank-2 formula to compute the 2-tangle,

$$\begin{aligned} \tau_{n,\eta} &= \sqrt{\text{Tr}(R) - \sqrt{2(\text{Tr}(R)^2 - \text{Tr}(R^2))}} \\ &= \sqrt{4w_\eta^2 w_n^2 + w_n^2 \sum_{(k_\eta=1)} b_k^2 - \sqrt{w_n^4 (\sum_{(k_\eta=1)} b_k^2)^2}} \\ &= 2w_\eta w_n. \end{aligned} \quad (2.42)$$

The one-party marginal has the matrix,

$$\begin{aligned}\rho_n &= \text{Tr}_{\hat{n}, n-1, \dots, 1} |\Psi\rangle \langle \Psi| \\ &= \begin{pmatrix} \sum_{(j < n)} w_j^2 + \sum_k b_k^2 + c^2 & w_n c \\ w_n c & w_n^2 \end{pmatrix},\end{aligned}\quad (2.43)$$

where the 1-tangle is given by twice the root of the determinant. Thus, we have the following n -tuple,

$$(\tau_{n|1}, \dots, \tau_{n|n-1}, \tau_n) = \left(2w_n w_1, \dots, 2w_n w_{n-1}, 2w_n \sqrt{\sum_{j < n} w_j^2 + \sum_k b_k^2} \right). \quad (2.44)$$

To see that this gives the solid hypercone defined by the monogamy relation, we will invert. Since c does not appear we will set it to zero as we will not need it. Clearly the expressions satisfy the relation,

$$\sum_k b_k^2 = (\tau_n^2 - \sum_j \tau_{n|j}^2) / 4w_n^2, \quad (2.45)$$

and the w_j 's are given by,

$$w_j^2 = \tau_{n|j}^2 / 4w_n^2, \quad (2.46)$$

for $j < n$ and finally from normalization we get the last parameter,

$$w_n^2 = \frac{1}{2} \left(1 \pm \sqrt{1 - \tau_n^2} \right). \quad (2.47)$$

Thus as long as Eq. 2.38 holds, we can find parameters that give the proper n -tuple.

Now consider a 3-tangle version of weak monogamy,

$$\tau_A^2 \geq \sum_{|I_A|=3} \tau_{I_A}^2, \quad (2.48)$$

where now only 3-tangles appear on the right. We can't comment on the necessity of this relation, but in 4-qubits the following states achieve equality,

$$|\psi\rangle_{ABCD} = a|0001\rangle + b|0010\rangle + c|0100\rangle + d|0111\rangle + q|1111\rangle, \quad (2.49)$$

with $a, b, c, d, q \geq 0$. To compute the mixed 3-tangles, recall that all the pure state decompositions of mixed states can be parametrized by a unitary [5] (the process to do so is described in more detail at the end of the next chapter), in turn, the 3-tangle roof points are parametrized as,

$$\tau_{A|B|C} = 2 \sum_k \sqrt{|U_{k,0}|^4 a^2 q^2}, \quad (2.50)$$

where U is any $K \times 2$ unitary matrix, K arbitrary, but then all unitary dependence gets wiped away since $\sum_k \sqrt{|U_{k,0}|^4} = 1$, so all decompositions have the same average 3-tangle. The other mixed 3-tangles follow the same pattern, thus our 4-tuple is,

$$(\tau_{A|B|C}, \tau_{A|B|D}, \tau_{A|C|D}, \tau_A) = (2aq, 2bq, 2cq, 2\sqrt{q^2(a^2 + b^2 + c^2)}). \quad (2.51)$$

Also note that the 2-tangles all vanish, therefore these states trivially satisfy the strong monogamy equality as well.

Chapter 2, in part, is currently being prepared for submission for publication of the material as, G. W. Allen, O. Bucicovschi, and D. A. Meyer, "Entanglement Constraints on States Locally Connected to the Greenberger-Horne-Zeilinger State." The dissertation author is a primary investigator and author of this paper.

Chapter 3

The Negativity Constrained: Explorations with d -level Systems

The prototypical quantum correlation, entanglement, is accountable for many of the effects seen in quantum theory, and there is a significant effort to enslave it as a resource to be manipulated and exploited by quantum engineers [7]. The most striking property of entanglement is its distributability, or lack thereof, exemplified by its compliance with, for example, monogamy laws [14] (as in Chapter 2) as well as area laws [58], laws which constrain the shareability of correlations. The former law states: the closer two parties are to being maximally entangled, the more the pair become separated and hidden from all other parties. The latter law: for certain types of many-particle ground states split in twain, the entanglement between the parts scales according to the size of the separation boundary. Both laws set the stage for entanglement to play a central role in physics, and an active research community continues to strengthen this role [59].

The secludedness of maximally entangled states has specifically impacted quantum key distribution [60], ground state frustration [61], and even black holes [62]. These

perspectives on monogamy have traditionally been understood in terms of multi-qubit networks. In the case of tripartite systems, the monogamy law can be written in terms of tangle [13] (also known as the concurrence), as the following,

$$\tau_{A|BC}^2 \geq \tau_{A|B}^2 + \tau_{A|C}^2, \quad (3.1)$$

where τ is the 2-tangle, subscripts label the parties, and the vertical bar denotes the bipartite split, and $\tau_{A|BC} = \tau_A$ is the 1-tangle (this equation is a immediate consequence Eq. 2.1). In this way, if $\tau_{A|BC}^2 \approx \tau_{A|B}^2 \approx 1$, i.e., A and B are maximally entangled, then $\tau_{A|C}^2 \approx 0$, hence the personification of entanglement.

The elegance and simplicity of the monogamy inequality has made it the paragon for entanglement shareability. It has since been shown that other entanglement measures such as, entanglement of formation [16], squashed entanglement [17], and entanglement negativity [18], all satisfy the same monogamy relation. This raises two issues: the monogamy inequality may just be a first order approximation to the shareability of correlational resources, so to what extent can we quantify the exact amount possible to share? Further, is the limited shareability a consequence of limited systems, i.e., qubits?

In any application of monogamy, it is then important to note that the law being satisfied does not necessarily imply its physical achievability. The 2-tangle is an exception to this rule: consider the achievable set of triples, $(\tau_{A|C}^2, \tau_{A|B}^2, \tau_{A|BC}^2)$, computed for all pure states of 3 qubits. The equality in Eq. 3.1 then defines a plane in the ambient space, $[0, 1]^3$. The original work [13] found saturation with the W class of states, $|W\rangle = a|001\rangle + b|010\rangle + c|100\rangle$, which do, in fact, map onto the entire plane in $[0, 1]^3$. Less well-known is the fact that the entire region above the plane can be achieved; see Fig. 3.1.

Entanglement negativity is not an exception to the above achievability rule. One

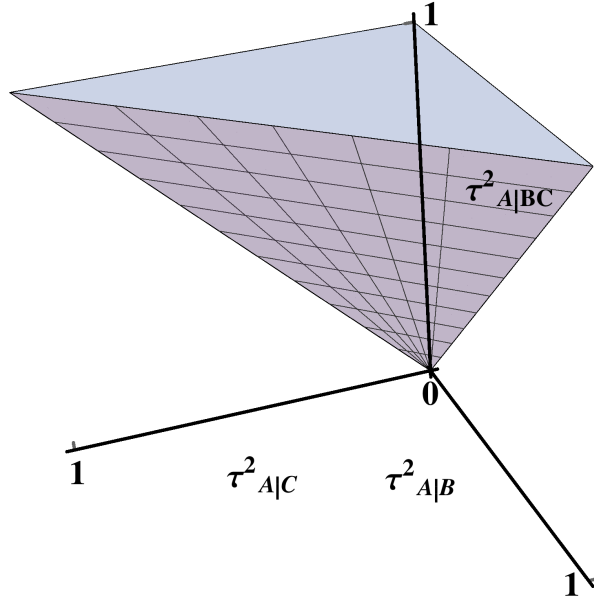


Figure 3.1: Achievable qubit tangles.

aim of this chapter is to make the fine print of its monogamy law legible; in other words, to derive the boundary of achievable correlations for negativity. Negativity, in particular, is important for several reasons. It is directly related to PPT states, a peculiar set of entangled states that, among other properties [63], cannot be distilled [64], so that negativity may be measuring “useful” entanglement. Further, negativity provides an alternative measure of mixed state entanglement that has the extremely rare property of being computable, indeed for *arbitrary* dimensional quantum system.

Recent advances in quantum photonics have allowed large dimensional subsystems to become commonplace [65]. There has even been a confirmation of entanglement between $D = 100$ dimensional qudits [66]. The need for a better understanding of correlations in these systems has arrived and negativity is one route to fulfill it. Negativity further rears its head in the study of gaussian states and continuous variable entanglement [67]. Therefore, another aim of this chapter is to touch on large quantum systems, in which we give a lower bound to the achievability boundary in all dimensions. Numerical evidence suggests it to be the upper bound as well.

3.1 Three Qubits

Negativity is based on the failure of the transpose operation to preserve positivity when acting on subsystems [64]. Transposing a separated system leaves the positivity unaffected, so a state with a non-positive partial transpose must be entangled. Negativity is defined as twice the sum of the negative eigenvalues of the partially transposed state:

$$\mathcal{N}_{A|B} = \mathcal{N}(\rho_{AB}) = 2 \sum_n \lambda_n^{(-)}(\rho_{AB}^{T_A}), \quad (3.2)$$

where $\rho_{AB}^{T_A}$ is the density matrix with the A tensor factor transposed. Although negativity is not obtained by a minimization procedure, it remarkably has many properties expected of an entanglement measure, *e.g.*, it has an interpretation as a distance to a separable state [68]. One can straightforwardly verify that for pure 2×2 systems, negativity and tangle agree, $\mathcal{N} = \tau$, and due to the convexity of negativity [64], the monogamy inequality for negativity immediately follows.

In order to find the tighter monogamy inequality, *i.e.*, the boundary of the achievable set $(\mathcal{N}_{A|C}^2, \mathcal{N}_{A|B}^2, \mathcal{N}_{A|BC}^2)$, it will be useful to have a parametrization for the 3-qubit pure states. Acín *et al.* showed how to “rotate out” all local unitaries to achieve a canonical form—a tripartite analog to Schmidt decomposition for pure bipartite states [43]. One such form is given as,

$$|\Psi\rangle = d|000\rangle + \omega|100\rangle + a|101\rangle + b|110\rangle + c|111\rangle, \quad (3.3)$$

with real $a, b, c, d \geq 0$, $\omega \in \mathbb{C}$, and the usual normalization (this equation can be recognized as a relabeling of Eq. 2.11). The boundary will be computed from “below” by maximizing the negativities in this parametrization.

Qubit negativity necessarily satisfies $0 \leq \mathcal{N} \leq 1$. We find the one-two party split

negativity straight forwardly,

$$\mathcal{N}_{A|BC}^2 = 4(a^2 + b^2 + c^2)d^2 = 4(1 - d^2 - |\omega|^2)d^2, \quad (3.4)$$

where the last equality follows from the normalization constraint. By maximizing with respect to d , we find the inequality, $0 \leq \mathcal{N}_{A|BC}^2 \leq (1 - |\omega|^2)^2$. Thus when $\mathcal{N}_{A|BC}^2$ is maximal, the parameter ω will vanish. For $\mathcal{N}_{A|BC}^2$ not maximal, it will be useful to consider for what values of ω are $\mathcal{N}_{A|C}^2$ and $\mathcal{N}_{A|B}^2$ both maximized.

To calculate $\mathcal{N}_{A|C}^2$, we need the following fact: a partial transpose cannot produce more than $(D - 1)^2$ negative eigenvalues for two entangled D -dimensional systems [69]. Accordingly, for two-qubit states, $\rho_{AC}^{T_A}$ has no more than one negative eigenvalue. The negativity is twice the negative eigenvalue, and thus satisfies the quartic polynomial equation,

$$\begin{aligned} 0 &= \det|2\rho_{AC}^{T_A} + \mathcal{N}_{A|C}I_4| \\ &= -16a^4d^4 - 16a^2c^2d^4 - 8a^4d^2x + 8a^2b^2d^2x \\ &\quad - 8a^2c^2d^2x - 8a^2d^4x - 8a^2d^2|\omega|^2x + 4a^2b^2x^2 \\ &\quad + 4b^2d^2x^2 + 4c^2d^2x^2 + 4c^2|\omega|^2x^2 + 2a^2x^3 \\ &\quad + 2b^2x^3 + 2c^2x^3 + 2|\omega|^2x^3 + x^4 \\ &\quad - (16d^2x + 8x^2)abc|\omega|\cos(\arg(\omega)), \end{aligned} \quad (3.5)$$

where I_4 is the 4×4 identity matrix and $x = \mathcal{N}_{A|C}$. Implicitly differentiating this quartic with respect to $\arg(\omega)$ and setting $\partial x / \partial(\arg(\omega)) = 0$ gives

$$8abc|\omega|x(2d^2 + x)\sin(\arg(\omega)) = 0, \quad (3.6)$$

so henceforth we restrict $\omega \in \mathbb{R}^+$ and drop the absolute value; the potential extra minus sign from $\omega \in \mathbb{R}^-$ does not affect the end result. Once again, differentiating the quartic in Eq. 3.5 with respect to ω and setting $\partial x / \partial \omega = 0$ gives

$$x(4abcd^2 + 4a^2d^2\omega + 2abcx - 2c^2\omega x - \omega x^2) = 0. \quad (3.7)$$

This gives one constraint, and along with normalization, leaves only three parameters. Since we are after a boundary surface in $[0, 1]^3$, we will eliminate another variable: Using Eq. 3.5 to maximize with respect to c gives:

$$8a^2cd^4 + 4a^2cd^2x + 4abd^2\omega x - 2cd^2x^2 + 2ab\omega x^2 - 2c\omega^2x^2 - cx^3 = 0. \quad (3.8)$$

Now we employ a powerful technique from computational algebraic geometry to perform algebraic elimination. Finding the minimal generating set, the *Gröbner basis*, for the ideal generated by these polynomial constraints [9], will give polynomials with the proper variables eliminated, as discussed in Chapter 1. The Gröbner basis for Eqs. 3.5 (with $\omega \in \mathbb{R}$), 3.7 and 3.8 has a single element; setting it to zero gives:

$$(2ad - x)(2a^2 + x)(2ad + x)(2d^2 + x)(2a^2d^2 + a^2x - b^2x)^2(4a^2d^2 - 2b^2x - x^2) = 0. \quad (3.9)$$

Neglecting negative solutions for x leaves three options: $x = 2ad$, and $x = -b^2 + \sqrt{b^4 + 4a^2d^2}$, the former producing a sub-manifold of the latter with $b = 0$. The solution $x = 2a^2d^2/(b^2 - a^2)$ also produces a sub-manifold: to show this, we now enforce normalization and find one more Gröbner basis. Eliminating x , ω , c , given the following constraints, $x = 2a^2d^2/(b^2 - a^2)$, Eqs. 3.5 (with $\omega \in \mathbb{R}$), 3.7, and normalization, produces,

$$a^7b^3d^4(a^2 - b^2 - ad)(a^2 - b^2 + ad)(-a^2 + b^2 + 2a^2d^2)^2 = 0, \quad (3.10)$$

demonstrating that $x = 2a^2d^2/(b^2 - a^2) = 2ad$ is again a sub-manifold of solution $x = -b^2 + \sqrt{b^4 + 4a^2d^2}$. A similar analysis on $\mathcal{N}_{A|B}^2$ leads to the following triples,

$$\begin{pmatrix} \mathcal{N}_{A|C}^2 \\ \mathcal{N}_{A|B}^2 \\ \mathcal{N}_{A|BC}^2 \end{pmatrix} = \begin{pmatrix} \left(b^2 - \sqrt{b^4 + 4a^2d^2}\right)^2 \\ \left(a^2 - \sqrt{a^4 + 4b^2d^2}\right)^2 \\ 4(a^2 + b^2)d^2 \end{pmatrix}. \quad (3.11)$$

These triples come from precisely the condition that $\omega = c = 0$, leaving states in Eq. 3.3 that are locally equivalent to the W class, the same class that maximize the 2-tangles. The three components of Eq. 3.11 parametrically define the boundary of the achievable set. Together with the normalization constraint, we can eliminate the state coefficients, turning the parametric surface into an implicit surface. Computing the Gröbner basis of the parametric polynomials, we again find a single element, which set to 0 gives the surface implicitly:

$$\begin{aligned} & z^6 - 2z^4(x^2 - xy + y^2) \\ & + z^2\left(x^4 + y^4 - 2xy(x(x-1) + y(y-1) - 3xy/2 + 2)\right) \\ & + xy(2y^2 + xy^2 + x^2y + 2x^2)(x + y + 2) = 0, \end{aligned} \quad (3.12)$$

where we identify $(x^2, y^2, z^2) \equiv (\mathcal{N}_{A|C}^2, \mathcal{N}_{A|B}^2, \mathcal{N}_{A|BC}^2)$.

We now show that Eq. 3.12 is the only non-trivial boundary of the achievable set. Adding back in the parameter c will fill in the rest of the set. The partially transposed reduced states are then full rank so that the determinants are negative as long as there is entanglement,

$$\begin{aligned} \det \rho_{A|C}^{T_A} &= -a^2d^4(a^2 + c^2), \\ \det \rho_{A|B}^{T_A} &= -b^2d^4(b^2 + c^2). \end{aligned} \quad (3.13)$$

Since $\mathcal{N}_{A|BC}^2 = 4(1 - d^2)d^2$, fixing z^2 will fix d . Thus, on a constant z^2 plane, starting at the boundary ($c = 0$), which is a curve intersecting the x^2z^2 - and y^2z^2 -coordinate planes at $(z^2, 0, z^2)$ and $(0, z^2, z^2)$, respectively, increasing c to $\sqrt{1 - d^2}$ will smoothly collapse the curve into the point $(0, 0, z^2)$ as a and b , and hence the determinants and the negativities, vanish. During this collapse, the curve continues to intersect the coordinate planes and traces out the achievable z^2 -plane set. As z^2 is arbitrary, all points between the boundary and the z^2 -axis can be achieved. See Fig. 3.2 for the achievable negativity set.

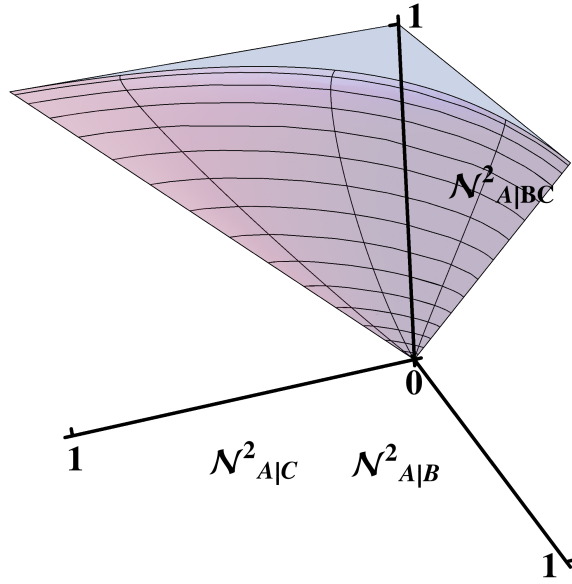


Figure 3.2: Achievable qubit negativity.

3.2 A New Monogamy Inequality

We would like to describe the achievable negativity set with a single inequality, as is done with achievable tangle set. It is not enough to modify Eq. 3.12 to be non-positive, simply due to the existence of multiple solutions $z = z(x, y)$, one of which intersects the achievable set's interior. We can factor out the unwanted solution with the following

coordinate transformation: $z \rightarrow 2\sqrt{\lambda(1-\lambda)}$. Plugging in to Eq. 3.12, the polynomial factors,

$$(8\lambda^3 - 16\lambda^2 + 2(x^2 + y^2 - xy + 4)\lambda - (2x^2 + 2y^2 + x^2y + xy^2)) \\ \times (8\lambda^3 - 8\lambda^2 + 2(x^2 + y^2 - xy)\lambda + (x^2y + xy^2 + 2xy)).$$

We take only the 2nd factor, and transform coordinates back, $\lambda \rightarrow \frac{1}{2}(1 + \sqrt{1 - z^2})$, which leaves us with the necessary and sufficient monogamy inequality for achievable negativities,

$$(z^2 - x^2 - y^2 + xy)(1 + \sqrt{1 - z^2}) - xy(2 + x + y) \geq 0. \quad (3.14)$$

3.3 Three Qudits

The states whose negativities fill up the region shown in Fig. 3.2 can be understood to have a special form, which is useful for generalizing this result to higher dimensional tensor factors. From Eq. 3.3 with $\omega = 0$,

$$|\Psi\rangle = d|000\rangle + a|101\rangle + b|110\rangle + c|111\rangle \\ = a|\Phi\rangle_{AC}|0\rangle_B + b|\Phi\rangle_{AB}|0\rangle_C + c|\text{GHZ}\rangle_{ABC} + (d - a - b - c)|000\rangle, \quad (3.15)$$

where $|\Phi\rangle = |00\rangle + |11\rangle$ and $|\text{GHZ}\rangle = |000\rangle + |111\rangle$. These states then generalize to D -dimensional qudits straightforwardly via $|\Phi\rangle \rightarrow \sum_j |jj\rangle$ and $|\text{GHZ}\rangle \rightarrow \sum_j |jjj\rangle$,

$$|\Psi\rangle = d|000\rangle + \sum_{j=1}^{D-1} a|j0j\rangle + b|jj0\rangle + c|jjj\rangle. \quad (3.16)$$

The partial transpose of the reduced density operator for Eq. 3.16 block diagonalizes to:

$$\rho_{A|C}^{T_A} = \left(d^2\right) \bigoplus_{j=1}^{\frac{(D-1)(D-2)}{2}} \begin{pmatrix} 0 & a^2 \\ a^2 & 0 \end{pmatrix} \bigoplus_{j=1}^{D-1} \begin{pmatrix} 0 & ad & 0 \\ ad & b^2 & bc \\ 0 & bc & a^2 + c^2 \end{pmatrix}. \quad (3.17)$$

$\rho_{A|B}^{T_A}$ has the same form with a and b interchanged. The similarity with the $D = 2$ case, particularly the 3×3 matrix factor, tells us that setting $c = 0$ maximizes the pairwise negativities for this family. The third negativity can be computed to be:

$$\mathcal{N}_{A|BC} = 2(D-1)d\sqrt{a^2 + b^2 + c^2} + (D-1)(D-2)(a^2 + b^2 + c^2), \quad (3.18)$$

so that again, fixing d will fix $\mathcal{N}_{A|BC}$. The same argument about the determinants applies again, so

$$\begin{aligned} \det \rho_{A|C}^{T_A} &= (-1)^{\lfloor \frac{D}{2} \rfloor} d^2 ((a^2 + c^2)d^2)^{(D-1)} a^{2(D-1)(D-2)} \\ \det \rho_{A|B}^{T_A} &= (-1)^{\lfloor \frac{D}{2} \rfloor} d^2 ((b^2 + c^2)d^2)^{(D-1)} b^{2(D-1)(D-2)}, \end{aligned} \quad (3.19)$$

on a constant $\mathcal{N}_{A|BC}$ -plane. And as before, increasing c to $\sqrt{(1-d^2)/(D-1)}$ will send a and b to 0 so the determinants, and thus the pairwise negativities, vanish. Since this is a natural extension of the achievable region we found for $D = 2$, we conjecture that it is the entire achievable set of negativities, $(\mathcal{N}_{A|C}^2, \mathcal{N}_{A|B}^2, \mathcal{N}_{A|BC}^2)$, for $D > 2$ as well.

For the boundary states ($c = 0$) the parameters can be eliminated for the Gröbner basis to get the conjectured implicit surface bound; however for any particular value of $D \geq 3$, the polynomial's complexity greatly increases, and therefore increases the difficulty of finding a single inequality to describe the set. For a generic value of D , the situation further takes a drastic turn, as we eliminate the state coefficients. For concreteness, we list the relevant polynomials,

$$\begin{aligned}
p_1 &= (b^4 + 4a^2d^2)(D-1)^2 - (x + b^2(D-1) - a^2(D-2)(D-1))^2, \\
p_2 &= (a^2 + 4b^2d^2)(D-1)^2 - (y + a^2(D-1) - b^2(D-2)(D-1))^2, \\
p_3 &= 4(a^2 + b^2)d^2(D-1)^2 - (z - (a^2 + b^2)(D-2)(D-1))^2, \\
p_4 &= (D-1)a^2 + (D-1)b^2 + d^2 - 1,
\end{aligned} \tag{3.20}$$

which come from re-writing the explicit expression of the $(x, y, z) \equiv (\mathcal{N}_{A|C}^2, \mathcal{N}_{A|B}^2, \mathcal{N}_{A|BC}^2)$ and the normalization condition. A Gröbner basis calculation does not complete in reasonable time, so we employ a different tool from elimination theory, the resultant (see Chapter 1). Using the normalization, we first eliminate d from p_1, p_2, p_3 , then compute $r_{12} = \text{Res}_d(p_1, p_2)$, and $r_{13} = \text{Res}_d(p_1, p_3)$, and finally computing $\text{Res}_b(r_{12}, r_{13})$, returns a polynomial with a, b, d eliminated, and thus by taking the correct factor of the calculated polynomial, it describes the conjectured boundary for arbitrary D . An explicit expression contains 1047 terms.

It is worth mentioning that naïvely testing the conjecture numerically is nearly hopeless, since the negativities of random states are highly non-uniform throughout the achievable set [70]. Nevertheless, testing for perturbations of our boundary, *via* superposition with a random state from the Haar measure, has led to no counter-examples.

An alternative way to derive our boundary states is the following. Consider the class of maximally entangled states between A and B , with an ancillary qudit, C ,

$$|\Psi\rangle = \left(d|00\rangle + \sum_{j=1}^{D-1} b|jj\rangle \right) |0\rangle. \tag{3.21}$$

These states give the entire line, $\mathcal{N}_{A|B} = \mathcal{N}_{A|BC}$ with $\mathcal{N}_{A|C} = 0$. Furthermore, given the

two-qudit swap Hamiltonian,

$$H_{\text{SWAP}} = \bigoplus_{j \leq k} \sigma_x^{(jk)}, \quad (3.22)$$

where $\sigma_x^{(jk)}$ is σ_x acting in the $\{j, k\}$ -subspace (unless $j = k$ in which case it is just 1 acting on the $\{j\}$ -subspace), let it act on the B and C qudits in Eq. 3.21:

$$e^{i\theta H_{\text{SWAP}}} |\Psi\rangle = d e^{i\theta} |000\rangle + b \sum_{j=1}^{D-1} \cos(\theta) |jj0\rangle + i \sin(\theta) |j0j\rangle. \quad (3.23)$$

Then the phases can be cleaned up with local unitaries to match Eq. 3.16, with $c = 0$.

3.4 Connections to Marginal Eigenvalues

Note that the boundary states Eq. 3.23 produce a surface that extends and folds back into the achievable set depending on the value of d , i.e., only maximizing the pairwise negativities when $d > 1/\sqrt{D}$, as seen from parametrically plotting the resulting polynomial surface in Fig. 3.3. Recall that negativity for $D \times D$ systems has bounds $0 \leq \mathcal{N} \leq D - 1$ [44].

The condition on d is related to conditions on the marginal eigenvalues: Higuchi found a necessary condition on the univariate marginal eigenvalues for pure N -qudit systems [71]; for three qudits it is,

$$\sum_{n=1}^{D-1} \lambda_n^{(A)} \leq \sum_{n=1}^{D-1} \lambda_n^{(B)} + \sum_{n=1}^{D-1} \lambda_n^{(C)}, \quad (3.24)$$

including permutations of the parties, where $\lambda_n^{(P)} \leq \lambda_{n+1}^{(P)}$, $n \in \{1, \dots, D-1\}$ are the ascending eigenvalues of party P 's state. The marginal eigenvalues of Eq. 3.16 with $c = 0$

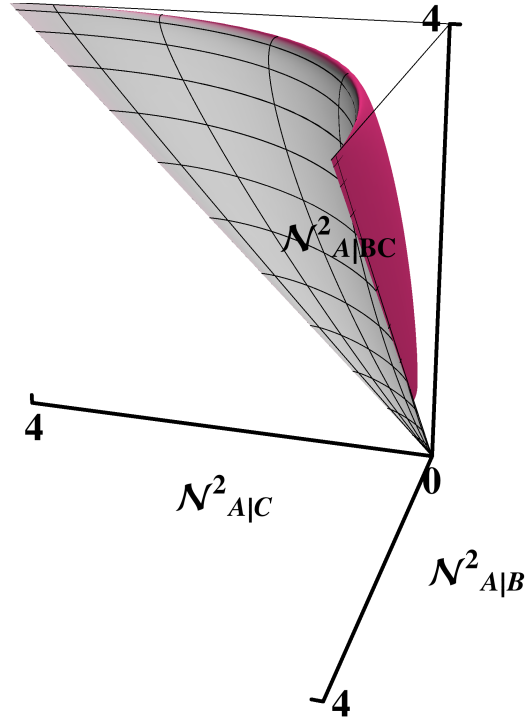


Figure 3.3: Achieved $D = 3$ negativity of states in Eq. 3.23. Red indicates the (nonbounding) part of the polynomial surface for $d < 1/\sqrt{D}$.

are

$$\lambda^{(A)} = \{(a^2 + b^2)_{(D-1)}, d^2\} \quad (3.25)$$

$$\lambda^{(B)} = \{(b^2)_{(D-1)}, (D-1)a^2 + d^2\} \quad (3.26)$$

$$\lambda^{(C)} = \{(a^2)_{(D-1)}, (D-1)b^2 + d^2\}, \quad (3.27)$$

where the subscripts denote the degeneracy. When $d > 1/\sqrt{D}$, the remaining, smaller, eigenvalues saturate the marginal inequality:

$$(D-1)(a^2 + b^2) \leq (D-1)a^2 + (D-1)b^2. \quad (3.28)$$

The expressions for the negativities are similar, to leading order in D :

$$\begin{pmatrix} \mathcal{N}_{A|C} \\ \mathcal{N}_{A|B} \\ \mathcal{N}_{A|BC} \end{pmatrix} = D^2 \begin{pmatrix} a^2 \\ b^2 \\ a^2 + b^2 \end{pmatrix} + O(D). \quad (3.29)$$

If our conjecture about achievable negativities is true, then in the limit of large dimensions, the monogamy inequality simplifies to

$$\mathcal{N}_{A|BC} \geq \mathcal{N}_{A|B} + \mathcal{N}_{A|C}, \quad (3.30)$$

up to terms of $O(1/D)$. See Fig. 3.4 for the achievable negativities *without squares*, $(\mathcal{N}_{A|C}, \mathcal{N}_{A|B}, \mathcal{N}_{A|BC})$.

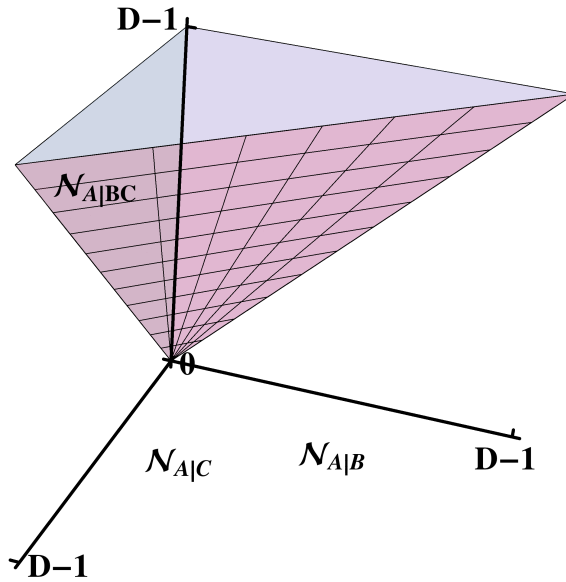


Figure 3.4: Achievable $D \rightarrow \infty$ negativity of states Eq. 3.16.

In summary, we've seen that although negativity is not itself a polynomial invariant in the state coefficients, the qubit negativity satisfies a polynomial equation. Simple maximization procedures combined with application of Gröbner basis computations (*i.e.*,

tools from Chapter 1) enabled us to derive an explicit expression for the boundary of the achievable set, a polynomial surface. Generalizing the qubit boundary states motivated a conjecture for the boundary of the achievable set for arbitrary dimensional qudits, a conjecture supported by numerical experimentation. We expect our approach to qubits to be relevant in proving the conjecture for qutrits, provided the proper 3-qutrit canonical form is found. For arbitrary dimensions we suspect an intimate connection with marginal eigenvalue constraints since our boundary states saturate the eigenvalue boundaries.

3.5 Convex Roof Extended Negativity

One of the largest drawbacks of using negativity, is that it doesn't always confirm the presence of entanglement, *i.e.*, the negativity evaluates to zero on some entangled states, called bound entangled states. This fact has motivated some authors to consider instead, the convex roof extended negativity. Since negativity on pure states of $D \times D$ bipartite states gives the pairwise product sum of the Schmidt coefficients,

$$\mathcal{N} \left(\sum_k \lambda_k |kk\rangle \right) = 2 \sum_{k=0}^{D-2} \sum_{k'=k+1}^{D-1} \lambda_k \lambda_{k'}, \quad (3.31)$$

it is faithful on pure states as only a product state would have a single non-zero Schmidt coefficient.

Here we make note that the boundary states of this chapter, Eq. 3.16, with $c = 0$, admit a tractable formula for the convex roof negativity. First we'll need the marginal, and the eigen-decomposition is readily found,

$$\rho_{A|B} = \left(d|00\rangle + \sum_j b|jj\rangle \right) \left(d\langle 00| + \sum_k b\langle kk| \right) + \sum_m a|m0\rangle \langle m0|. \quad (3.32)$$

Now every pure state decomposition can be obtained by a unitary matrix, [5], with the

following construction on some density matrix, ρ ,

$$\begin{aligned}
\rho &= \sum_i \lambda_i |\psi_i\rangle \langle \psi_i| \\
&= \sum_i \sqrt{\lambda_i} |\psi_i\rangle \langle \psi_i| \sqrt{\lambda_i} \\
&= \sum_{i,j} \delta_{i,j} \sqrt{\lambda_i} |\psi_i\rangle \langle \psi_j| \sqrt{\lambda_j} \\
&= \sum_{i,j,k} U_{i,k} \sqrt{\lambda_i} |\psi_i\rangle \langle \psi_j| \sqrt{\lambda_j} U_{k,j}^\dagger \\
&= \sum_k \left(\sum_i U_{i,k} \sqrt{\lambda_i} |\psi_i\rangle \right) \left(\sum_j \langle \psi_j| \sqrt{\lambda_j} U_{j,k}^* \right) \\
&= \sum_k |z^{(k)}\rangle \langle z^{(k)}|,
\end{aligned} \tag{3.33}$$

with the unnormalized states defined as, $|z^{(k)}\rangle = \sum_i U_{i,k} \sqrt{\lambda_i} |\psi_i\rangle$. Applying this formula to our marginal in Eq. 3.32, gives,

$$|z^{(k)}\rangle = U_{0,k} d |00\rangle + \sum_{j \geq 1} U_{0,k} b |jj\rangle + \sum_{m \geq 1} U_{m,k} a |m0\rangle. \tag{3.34}$$

To find the negativity of this state, we want to compute the Schmidt coefficients. Letting $|z^{(k)}\rangle = \sum_{i,j} z_{i,j}^{(k)} |i, j\rangle$, then we compute the singular values of the matrix operator formed by the coefficients, $z^{(k)} = \sum_{i,j} z_{i,j}^{(k)} |i\rangle \langle j|$ and thus the eigenvalues of the following $D \times D$ operator,

$$\begin{aligned}
z^{(k)\dagger} z^{(k)} &= \left(|U_{0,k}|^2 d^2 + \sum_{m \geq 1} |U_{m,k}|^2 a^2 \right) |0\rangle \langle 0| + \sum_{j \geq 1} |U_{0,k}|^2 b^2 |j\rangle \langle j| \\
&\quad + \sum_{m \geq 1} U_{0,k} U_{m,k}^* a b |0\rangle \langle m| + U_{0,k}^* U_{m,k} a b |m\rangle \langle 0|.
\end{aligned} \tag{3.35}$$

It is easy to pick off eigenvalues using the last $D - 1$ columns with eigenvectors of the form, $|e_i\rangle = U_{i,k}^* |1\rangle - U_{1,k}^* |i\rangle$ with $i = 2, \dots, D - 1$, which all correspond to the

same eigenvalue, the square of a Schmidt coefficient, $\lambda_0^2 = |U_{0,k}|^2 b^2$. For the last two eigenvalues, it will be easier to calculate if we remove the diagonal. In that case we use the eigenvector ansatz, $|e_{\pm}\rangle = \Lambda|0\rangle + \sum_{m \geq 1} U_{0,k}^* U_{m,k} a b |m\rangle$, for some unknown Λ , and we get,

$$\begin{aligned}
& \left(z^{(k)\dagger} z^{(k)} - |U_{0,k}|^2 b^2 I_D \right) |e_{\pm}\rangle \\
&= \left(-|U_{0,k}|^2 b^2 \Lambda + |U_{0,k}|^2 d^2 \Lambda + \sum_{m \geq 1} |U_{m,k}|^2 a^2 \Lambda + \sum_{m \geq 1} |U_{0,k}|^2 |U_{m,k}|^2 a^2 b^2 \right) |0\rangle \\
&\quad + \sum_{m \geq 1} U_{0,k}^* U_{m,k} a b \Lambda |m\rangle \\
&\stackrel{?}{=} \Lambda |e_{\pm}\rangle.
\end{aligned} \tag{3.36}$$

In order to get the last equality, we need the coefficient of $|0\rangle$ to match on both sides,

$$\left(-|U_{0,k}|^2 b^2 \Lambda + |U_{0,k}|^2 d^2 \Lambda + \sum_{m \geq 1} |U_{m,k}|^2 a^2 \Lambda + \sum_{m \geq 1} |U_{0,k}|^2 |U_{m,k}|^2 a^2 b^2 \right) = \Lambda^2. \tag{3.37}$$

The parameter Λ is the eigenvalue of $\left(z^{(k)\dagger} z^{(k)} - |U_{0,k}|^2 b^2 I_D \right)$, so we need to add $|U_{0,k}|^2 b^2$ to Λ to get the eigenvalue of $z^{(k)\dagger} z^{(k)}$, which is still the square of the Schmidt coefficient, which we get,

$$\begin{aligned}
\lambda_{\pm}^2 &= \Lambda + |U_{0,k}|^2 b^2 = \\
&= \frac{1}{2} \left(|U_{0,k}|^2 b^2 + |U_{0,k}|^2 d^2 + \sum_{m \geq 1} |U_{m,k}|^2 a^2 \right. \\
&\quad \left. \pm \sqrt{\left(-|U_{0,k}|^2 b^2 + |U_{0,k}|^2 d^2 + \sum_{m \geq 1} |U_{m,k}|^2 a^2 \right)^2 + 4 \sum_{m \geq 1} |U_{0,k}|^2 |U_{m,k}|^2 a^2 b^2} \right).
\end{aligned} \tag{3.38}$$

Since there are only three distinct Schmidt coefficients, the negativity becomes, from

Eq. 3.31,

$$\mathcal{N}(|z^{(k)}\rangle) = (D-2)(D-3)\lambda_0^2 + 2(D-1)\lambda_0(\lambda_+ + \lambda_-) + 2\lambda_+\lambda_-. \quad (3.39)$$

Some significant simplification happens,

$$\lambda_+\lambda_- = |U_{0,k}|^2 bd, \quad (3.40)$$

and

$$\begin{aligned} \lambda_0(\lambda_+ + \lambda_-) &= \lambda_0 \sqrt{\lambda_+^2 + \lambda_-^2 + 2\lambda_+\lambda_-} \\ &= |U_{0,k}|b \sqrt{|U_{0,k}|^2(b+d)^2 + \sum_{m \geq 1} |U_{m,k}|^2 a^2}. \end{aligned} \quad (3.41)$$

Note, in preparation for evaluating the convex roof, we'll be looking for a U that will minimize the above, and we can get a head start by choosing a U that satisfies, $|U_{0,k}||U_{m,k}| = 0$, so that for the k th the column, 0th row can only have non-zero elements when the m th row elements are zero, and *vice versa*. This choice simplifies the above to,

$$\lambda_0(\lambda_+ + \lambda_-) = |U_{0,k}|^2 b(b+d). \quad (3.42)$$

Now the roof points of the negativity of ρ_{AB} , with the above choice of U are,

$$\begin{aligned}
& \mathcal{N} \left(\left\{ \langle z^{(k)} | z^{(k)} \rangle, \frac{|z^{(k)}\rangle}{\sqrt{\langle z^{(k)} | z^{(k)} \rangle}} \right\} \right) \\
&= \sum_k \langle z^{(k)} | z^{(k)} \rangle \mathcal{N} \left(\frac{|z^{(k)}\rangle \langle z^{(k)}|}{\langle z^{(k)} | z^{(k)} \rangle} \right) \\
&= \sum_k \mathcal{N} \left(|z^{(k)}\rangle \langle z^{(k)}| \right) \\
&= \sum_k |U_{0,k}|^2 ((D-2)(D-2)b^2 + 2(D-1)b(b+d) + 2bd) \\
&= (D-2)(D-2)b^2 + 2(D-1)b(b+d) + 2bd \\
&= (D-1) ((D-2)b^2 + 2bd),
\end{aligned} \tag{3.43}$$

where the 3rd line follows since negativity is homogeneous, and the unitary matrix obeys the normalization condition $\sum_k |U_{0,k}|^2 = 1$. Note that these expressions could result from the eigen-decomposition which shows that such a decomposition is in this case, optimal. Hence the convex roof negativities of our boundary states are,

$$\begin{aligned}
\check{\mathcal{N}}_{AB} &= (D-1) ((D-2)b^2 + 2bd), \\
\check{\mathcal{N}}_{AC} &= (D-1) ((D-2)a^2 + 2ad).
\end{aligned} \tag{3.44}$$

See Fig 3.5 for a plot of these convex roof negativities vs the non-roof negativities for 4-level systems. Recall that negativity is a convex function, and the convex roof is the maximal convex function coinciding with its definition on pure states, so we always have, $\mathcal{N} \leq \check{\mathcal{N}}$.

From the plot it appears that these states do not violate the CKW type inequality for convex roof negativity, $\check{\mathcal{N}}_{A|BC}^2 \geq \check{\mathcal{N}}_{A|C}^2 + \check{\mathcal{N}}_{A|B}^2$. And finally, one can see from the parametrizations, Eq. 3.44, in the limit of large dimensions, these states also satisfy the

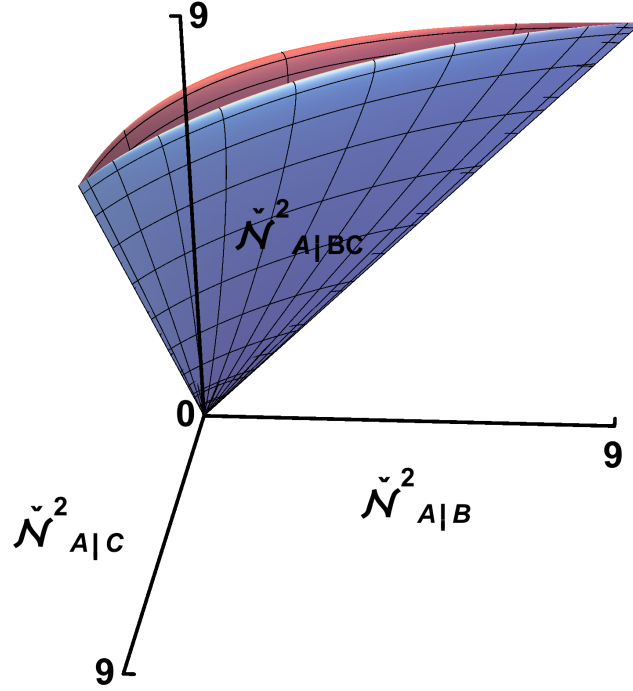


Figure 3.5: Achieved $D = 4$ convex roof negativity of states in Eq. 3.23. The blue surface is the parametrized surface from expressions Eq. 3.44 for $d < 1/\sqrt{D}$, and for comparison, the red surface is the regular non-roof negativities of the same states.

same relation as non-roof negativities,

$$\check{\mathcal{N}}_{A|BC} = \check{\mathcal{N}}_{A|B} + \check{\mathcal{N}}_{A|C}, \quad (3.45)$$

up to terms of $O(1/D)$.

Chapter 3, in large part, is a reprint of the material as it appears in G. W. Allen and D. A. Meyer, “Polynomial Monogamy Relations for Entanglement Negativity,” Phys. Rev. Lett. 118, 080402 (2017). The dissertation author was a primary investigator and author of this paper.

Chapter 4

The Comparisons Continue:

Explorations with the Globally Mixed

16 years ago, an early comparison of negativity and the 2-tangle [72] showed that on 2-qubit mixed states for a fixed value of the tangle, τ , the following negativities, $\mathcal{N}$, are possible,

$$\sqrt{(1-\tau)^2 + \tau^2} - (1-\tau) \leq \mathcal{N} \leq \tau. \quad (4.1)$$

This result alone implied that negativity must be monogamous if the 2-tangle is. In the last chapter, it was found that the negativity monogamy triple of three parties, $(\mathcal{N}_{A|BC}, \mathcal{N}_{AC}, \mathcal{N}_{AB})$, is even more tightly constrained than that implied by the above equation [56] — the two measures are constrained in the multipartite setting by algebraically different relations,

$$\begin{aligned} \tau_{A|BC}^2 - \tau_{AB}^2 - \tau_{AC}^2 &\geq 0, \\ \left(\mathcal{N}_{A|BC}^2 - \mathcal{N}_{AB}^2 - \mathcal{N}_{AC}^2 + \mathcal{N}_{AB}\mathcal{N}_{AC} \right) \left(1 + \sqrt{1 - \mathcal{N}_{A|BC}^2} \right) - \mathcal{N}_{AB}\mathcal{N}_{AC}(2 + \mathcal{N}_{AB} + \mathcal{N}_{AC}) &\geq 0. \end{aligned} \quad (4.2)$$

In the theory of entanglement constraints, the monogamy relations play a dominant role, especially since different entanglement measures appear to satisfy monogamy-like relations. On the other hand, another recent result [45] found symmetrical constraints on 3-qubit pure state 2-tangle triples $(\tau_{BC}, \tau_{AC}, \tau_{AB})$,

$$\begin{aligned}
& 1 - \tau_{BC}^2 - \tau_{AC}^2 - \tau_{AB}^2 \\
& + \sqrt{(1 - \tau_{BC} - \tau_{AC} + \tau_{AB})(1 - \tau_{BC} + \tau_{AC} - \tau_{AB})} \\
& \times \sqrt{(1 + \tau_{BC} - \tau_{AC} - \tau_{AB})(1 + \tau_{BC} + \tau_{AC} - \tau_{AB})} \geq 0.
\end{aligned} \tag{4.3}$$

Unlike the monogamy relation on the tangles, Eq. 4.2 which remains valid for arbitrary 3-qubit mixed states, the above party-symmetric constraint is actually violated on mixed states. In a sense then, we find a striking counter-intuitive phenomena — sometimes classical uncertainty can force the quantum states to become *more* entangled, but in such a way that doesn't affect the monogamy-type sharing. Before we get to that, we would first like to continue the trend of finding the corresponding party-symmetric constraints on negativity.

4.1 Party-Symmetric Negativities

As usual (as seen in Chapter 2 and Chapter 3), it is convenient to work in the 3-qubit Schmidt form [43], given by

$$\Psi = (a_0, a_1, a_2, a_3, a_4, a_5, a_6, a_7) \xrightarrow{U_A \otimes U_B \otimes U_C} (\lambda_0, 0, 0, 0, \lambda_1 e^{i\varphi}, \lambda_2, \lambda_3, \lambda_4), \tag{4.4}$$

with real parameters $(\lambda_0, \lambda_1, \lambda_2, \lambda_3, \lambda_4, \varphi) \geq 0$. An algebraically simpler and (almost) complete set of unitary invariants is given by,

$$\begin{aligned}
J_1 &= \tau_{BC}^2/4 = |\lambda_2\lambda_3 - e^{i\varphi}\lambda_1\lambda_4|^2, \\
J_2 &= \tau_{AC}^2/4 = \lambda_0^2\lambda_2^2, \\
J_3 &= \tau_{AB}^2/4 = \lambda_0^2\lambda_3^2, \\
J_4 &= \tau_{ABC}^2/4 = \lambda_0^2\lambda_4^2, \\
J_5 &= 2\sqrt{J_2J_3}(\lambda_2\lambda_3 - \lambda_1\lambda_4\cos(\varphi)).
\end{aligned} \tag{4.5}$$

Negativity is a unitary invariant, so it must be algebraically dependent on the above invariants; it is determined by the zero of the characteristic equation, $\det(2\rho_{AC}^{T_A} + \mathcal{N}_{AC}I_4) = 0$, written out as,

$$\mathcal{N}_{AC}^4 + 2\mathcal{N}_{AC}^3 + 4\mathcal{N}_{AC}^2(J_1 + J_3 + J_4) + 8\mathcal{N}_{AC}(J_5 - J_2) - 16J_2(J_2 + J_4) = 0. \tag{4.6}$$

We are interested in extreme values of negativity, and it is convenient to extremize with respect to φ ,

$$\begin{aligned}
&\partial_\varphi \det(2\rho_{AC}^{T_A} + \mathcal{N}_{AC}I_4)|_{\partial_\varphi \mathcal{N}_{AC}=0} = 0 \\
&= 8\mathcal{N}_{AC}(\mathcal{N}_{AC} + 2\lambda_0^2)\lambda_1\lambda_2\lambda_3\lambda_4\sin(\varphi),
\end{aligned} \tag{4.7}$$

so we set, $\varphi = 0, \pi$. With either value of φ , one of the above invariants becomes dependent, $J_5 = \pm 2\sqrt{J_2J_3}$, which then implies that we have a map from $(\tau_{BC}, \tau_{AC}, \tau_{AB}, \tau_{ABC}) \mapsto (\mathcal{N}_{BC}, \mathcal{N}_{AC}, \mathcal{N}_{AB}, \tau_{ABC})$, which enables us to utilize a very special fact, that either: boundaries are mapped to boundaries, or a vanishing Jacobian determines the boundary (as explained in Chapter 1). The boundary of $(\tau_{BC}, \tau_{AC}, \tau_{AB}, \tau_{ABC})$ is known and is given by

the polynomial constraint,

$$(\tau_{ABC}^2 + \tau_{BC}\tau_{AC}\tau_{AB})^2 = (\tau_{ABC}^2 + \tau_{BC}^2)(\tau_{ABC}^2 + \tau_{AC}^2)(\tau_{ABC}^2 + \tau_{AB}^2). \quad (4.8)$$

States which satisfy this equation with $J_5 = \pm 2\sqrt{J_1 J_2 J_3}$, are necessarily and sufficiently given by type 4d in [43], which we call Thue-Morse states, states which have non-zero coefficients on computational basis states with an odd parity of ones [73],

$$\langle ijk|TM\rangle = (0, \sqrt{c}, \sqrt{b}, 0, \sqrt{a}, 0, 0, \sqrt{d}), \quad (4.9)$$

with $a, b, c, d \geq 0$ and $a + b + c + d = 1$. Note that these states have another nickname, X-states, as the two party marginals have the characteristic X-shaped density matrix. These states are mapped to the boundary of $(\mathcal{N}_{BC}, \mathcal{N}_{AC}, \mathcal{N}_{AB}, \tau_{ABC})$, and such a boundary can be used to find the boundary of $(\mathcal{N}_{BC}, \mathcal{N}_{AC}, \mathcal{N}_{AB})$ by projecting out τ_{ABC} , so then the Thue-Morse states can determine the boundary of the negativity triples. The negativities of Thue-Morse are computed to be,

$$\begin{pmatrix} \mathcal{N}_{BC} \\ \mathcal{N}_{AC} \\ \mathcal{N}_{AB} \end{pmatrix} = \begin{pmatrix} \sqrt{(d+a)^2 - 4(da-bc)} - (d+a) \\ \sqrt{(d+b)^2 - 4(db-ac)} - (d+b) \\ \sqrt{(d+c)^2 - 4(dc-ab)} - (d+c) \end{pmatrix}, \quad (4.10)$$

and we eliminate the parameters to find the boundary of negativities. First we eliminate $a = 1 - b - c - d$ from all the equations. Then take the first equation, which can be written as $f_1(\mathcal{N}_{BC}, a, b, c, d) = f_1(\mathcal{N}_{BC}, 1 - b - c - d, b, c, d) = 0$ and solve for b to substitute it into the other two equations, which take the form $f_2(\mathcal{N}_{AC}, \mathcal{N}_{BC}, c, d) = 0$ and $f_3(\mathcal{N}_{AB}, \mathcal{N}_{BC}, c, d) = 0$, where the f 's are all polynomial in the arguments. The easiest way to eliminate c is by taking the vanishing resultant (as discussed in Chapter 1), $\text{Res}_c(f_2, f_3) = 0 = f_4(\mathcal{N}_{BC}, \mathcal{N}_{AC}, \mathcal{N}_{AB}, d)$. Finally the boundary of triples $(\mathcal{N}_{BC}, \mathcal{N}_{AC}, \mathcal{N}_{AB})$

can be determined by projecting out d from the polynomial surface $f_4 = 0$. There are two boundaries which show up in the projection — one: from the discriminant of f_4 which gives the enveloping surface, and two: by setting $d = 0$, since d is real and positive and the enveloping surface from the discriminant would otherwise be blind to this constraint. The discriminant of f_4 with respect to d contains 362 terms and is given by,

$$\begin{aligned}
& -256 - 1024x - 768x^2 + 2048x^3 + 768x^8 - 2048x^7 - 3584x^6 + 3584x^4 \\
& + 256x^{10} + 1024x^9 - 4096xy - 1024y + 3072x^5y + 11264x^4y + 5120x^3y - 3840x^2y \\
& + 256x^{10}y + 1024x^9y - 5120x^7y - 6656x^6y + 12192x^3y^2 - 1824x^2y^2 - 3840xy^2 - 768y^2 \\
& - 3168x^7y^2 - 2592x^6y^2 + 8640x^5y^2 + 19776x^4y^2 - 768x^8y^2 + 12192x^2y^3 + 5120xy^3 \\
& + 2048y^3 + 192x^6y^3 + 10848x^5y^3 + 28448x^4y^3 + 27104x^3y^3 - 192x^7y^3 + 19776x^2y^4 \\
& + 11264xy^4 + 3584y^4 - 261x^6y^4 + 8118x^5y^4 + 24635x^4y^4 + 28448x^3y^4 - 96x^7y^4 \\
& + 10848x^3y^5 + 8640x^2y^5 + 3072xy^5 + 54x^6y^5 + 2892x^5y^5 + 8118x^4y^5 - 3584y^6 \\
& - 261x^4y^6 + 192x^3y^6 - 2592x^2y^6 - 6656xy^6 + 27x^6y^6 + 54x^5y^6 - 5120xy^7 - 2048y^7 \\
& - 96x^4y^7 - 192x^3y^7 - 3168x^2y^7 + 768y^8 - 768x^2y^8 + 1024xy^9 + 256y^{10} + 1024y^9 \\
& - 3840x^2z + 256xy^{10} - 4096xz - 1024z - 6656x^6z + 3072x^5z + 11264x^4z \\
& + 5120x^3z + 256x^{10}z + 1024x^9z - 5120x^7z - 4096yz + 24896x^4yz - 6208x^3yz \\
& - 33792x^2yz - 21760xyz - 1728x^8yz - 11840x^7yz - 13184x^6yz + 11136x^5yz + 256x^{10}yz \\
& + 1024x^9yz - 33792xy^2z - 3840y^2z + 18528x^5y^2z + 26208x^4y^2z - 28992x^3y^2z \\
& - 65856x^2y^2z - 1728x^8y^2z - 6816x^7y^2z - 5856x^6y^2z + 5120y^3z + 39584x^4y^3z \\
& + 1136x^3y^3z - 28992x^2y^3z - 6208xy^3z - 192x^7y^3z + 384x^6y^3z + 21360x^5y^3z + 11264y^4z \\
& + 43712x^4y^4z + 39584x^3y^4z + 26208x^2y^4z + 24896xy^4z - 96x^7y^4z - 288x^6y^4z \\
& + 16512x^5y^4z + 3072y^5z + 16512x^4y^5z + 21360x^3y^5z + 18528x^2y^5z + 11136xy^5z \\
& + 5616x^5y^5z - 5856x^2y^6z - 13184xy^6z - 6656y^6z - 288x^4y^6z + 384x^3y^6z - 11840xy^7z \\
& - 5120y^7z - 96x^4y^7z - 192x^3y^7z - 6816x^2y^7z - 1728xy^8z - 1728x^2y^8z + 1024xy^9z \\
& + 256y^{10}z + 1024y^9z - 1824x^2z^2 + 256xy^{10}z - 3840xz^2 - 768z^2 - 2592x^6z^2 + 8640x^5z^2 \\
& + 19776x^4z^2 + 12192x^3z^2 - 768x^8z^2 - 3168x^7z^2 - 33792xyz^2 - 3840yz^2 + 18528x^5yz^2 \\
& + 26208x^4yz^2 - 28992x^3yz^2 - 65856x^2yz^2 - 1728x^8yz^2 - 6816x^7yz^2 - 5856x^6yz^2 \\
& - 1824y^2z^2 - 14838x^4y^2z^2 - 135456x^3y^2z^2 - 169872x^2y^2z^2 - 65856xy^2z^2 - 960x^8y^2z^2 \\
& - 3648x^7y^2z^2 - 3654x^6y^2z^2 + 13812x^5y^2z^2 - 124848x^3y^3z^2 - 135456x^2y^3z^2 \\
& - 28992xy^3z^2 + 12192y^3z^2 - 390x^6y^3z^2 + 9540x^5y^3z^2 - 20646x^4y^3z^2 + 19776y^4z^2 \\
& + 9072x^4y^4z^2 - 20646x^3y^4z^2 - 14838x^2y^4z^2 + 26208xy^4z^2 + 8448x^5y^4z^2 + 13812x^2y^5z^2 \\
& + 18528xy^5z^2 + 8640y^5z^2 + 2832x^5y^5z^2 + 8448x^4y^5z^2 + 9540x^3y^5z^2 - 2592y^6z^2 \\
& - 390x^3y^6z^2 - 3654x^2y^6z^2 - 5856xy^6z^2 - 3168y^7z^2 - 3648x^2y^7z^2 - 1728xy^8z^2 \\
& - 6816xy^7z^2 - 768y^8z^2 - 960x^2y^8z^2 + 12192x^2z^3 + 5120xz^3 + 2048z^3 + 192x^6z^3 \\
& + 10848x^5z^3 + 28448x^4z^3 + 27104x^3z^3 - 192x^7z^3 - 28992x^2yz^3 - 6208xyz^3 + 5120yz^3 \\
& + 384x^6yz^3 + 21360x^5yz^3 + 39584x^4yz^3 + 1136x^3yz^3 - 192x^7yz^3 - 135456x^2y^2z^3 \\
& - 28992xy^2z^3 + 12192y^2z^3 - 390x^6y^2z^3 + 9540x^5y^2z^3 - 20646x^4y^2z^3 - 124848x^3y^2z^3 \\
& - 144452x^3y^3z^3 - 124848x^2y^3z^3 + 1136xy^3z^3 + 27104y^3z^3 - 582x^6y^3z^3 - 972x^5y^3z^3 \\
& - 45962x^4y^3z^3 + 28448y^4z^3 - 14180x^4y^4z^3 - 45962x^3y^4z^3 - 20646x^2y^4z^3 + 39584xy^4z^3
\end{aligned}$$

$$\begin{aligned}
& -972x^3y^5z^3 + 9540x^2y^5z^3 + 21360xy^5z^3 + 10848y^5z^3 - 582x^3y^6z^3 - 390x^2y^6z^3 \\
& + 384xy^6z^3 + 192y^6z^3 - 192xy^7z^3 + 11264xz^4 - 192y^7z^3 + 3584z^4 + 8118x^5z^4 \\
& + 24635x^4z^4 + 28448x^3z^4 + 19776x^2z^4 - 96x^7z^4 - 261x^6z^4 + 24896xyz^4 + 11264yz^4 \\
& + 16512x^5yz^4 + 43712x^4yz^4 + 39584x^3yz^4 + 26208x^2yz^4 - 96x^7yz^4 - 288x^6yz^4 \\
& + 26208xy^2z^4 + 19776y^2z^4 + 8448x^5y^2z^4 + 9072x^4y^2z^4 - 20646x^3y^2z^4 - 14838x^2y^2z^4 \\
& - 45962x^3y^3z^4 - 20646x^2y^3z^4 + 39584xy^3z^4 + 28448y^3z^4 - 14180x^4y^3z^4 + 9072x^2y^4z^4 \\
& + 43712xy^4z^4 + 24635y^4z^4 - 4148x^4y^4z^4 - 14180x^3y^4z^4 + 16512xy^5z^4 + 8118y^5z^4 \\
& + 8448x^2y^5z^4 - 288xy^6z^4 - 96y^7z^4 - 261y^6z^4 + 10848x^3z^5 + 8640x^2z^5 - 96xy^7z^4 \\
& + 3072xz^5 + 54x^6z^5 + 2892x^5z^5 + 8118x^4z^5 + 3072yz^5 + 16512x^4yz^5 + 21360x^3yz^5 \\
& + 18528x^2yz^5 + 11136xyz^5 + 5616x^5yz^5 + 13812x^2y^2z^5 + 18528xy^2z^5 + 8640y^2z^5 \\
& + 2832x^5y^2z^5 + 8448x^4y^2z^5 + 9540x^3y^2z^5 + 10848y^3z^5 - 972x^3y^3z^5 + 9540x^2y^3z^5 \\
& + 21360xy^3z^5 + 8118y^4z^5 + 8448x^2y^4z^5 + 5616xy^5z^5 + 16512xy^4z^5 + 2892y^5z^5 \\
& + 2832x^2y^5z^5 - 6656xz^6 + 54y^6z^5 - 3584z^6 + 54x^5z^6 - 261x^4z^6 + 192x^3z^6 - 2592x^2z^6 \\
& + 27x^6z^6 - 5856x^2yz^6 - 13184xyz^6 - 6656yz^6 - 288x^4yz^6 + 384x^3yz^6 - 5856xy^2z^6 \\
& - 2592y^2z^6 - 390x^3y^2z^6 - 3654x^2y^2z^6 + 384xy^3z^6 + 192y^3z^6 - 582x^3y^3z^6 - 390x^2y^3z^6 \\
& - 288xy^4z^6 - 261y^4z^6 - 5120xz^7 + 27y^6z^6 + 54y^5z^6 - 2048z^7 - 96x^4z^7 - 192x^3z^7 \\
& - 3168x^2z^7 - 5120yz^7 - 96x^4yz^7 - 192x^3yz^7 - 6816x^2yz^7 - 11840xyz^7 - 3648x^2y^2z^7 \\
& - 6816xy^2z^7 - 192y^3z^7 - 3168y^2z^7 - 96xy^4z^7 - 192xy^3z^7 - 96y^4z^7 + 768z^8 - 1728x^2yz^8 \\
& - 768x^2z^8 - 1728xyz^8 - 768y^2z^8 - 960x^2y^2z^8 - 1728xy^2z^8 + 1024xz^9 + 1024z^9 \\
& + 1024xyz^9 + 256xz^{10} + 1024yz^9 + 256z^{10} + 256xyz^{10} + 256yz^{10} = 0. \tag{4.11}
\end{aligned}$$

The other boundary, $f_4|_{d=0} = 0$ contains 72 terms and is given by,

$$\begin{aligned}
& -x^6y^2 - 2x^5y^2 - 2x^4y^3 - 4x^3y^3 - 2x^4y^4 - 2x^3y^4 - x^2y^6 - 2x^2y^5 - 16x^4yz - 32x^3yz \\
& + 16x^2yz + 32xyz + 2x^6yz + 4x^5yz - 8x^2y^2z + 16xy^2z - 14x^4y^2z - 36x^3y^2z - 36x^2y^3z \\
& - 32xy^3z + 2x^4y^3z - 4x^3y^3z - 14x^2y^4z - 16xy^4z - 2x^5z^2 + 2x^3y^4z + 2xy^6z + 4xy^5z - x^6z^2 \\
& - 36x^3yz^2 - 8x^2yz^2 + 16xyz^2 - 14x^4yz^2 - 52x^3y^2z^2 - 52x^2y^2z^2 - 8xy^2z^2 - 16x^4y^2z^2 \\
& - 10x^3y^3z^2 - 52x^2y^3z^2 - 36xy^3z^2 - 16x^2y^4z^2 - 14xy^4z^2 - y^6z^2 - 2y^5z^2 - 2x^4z^3 - 4x^3z^3 \\
& - 36x^2yz^3 - 32xyz^3 + 2x^4yz^3 - 4x^3yz^3 - 52x^2y^2z^3 - 36xy^2z^3 - 10x^3y^2z^3 - 10x^2y^3z^3 \\
& - 4xy^3z^3 - 4y^3z^3 - 2x^4z^4 - 2x^3z^4 + 2xy^4z^3 - 2y^4z^3 + 2x^3yz^4 - 14x^2yz^4 - 14xy^2z^4 - 16xyz^4 \\
& - 16x^2y^2z^4 + 2xy^3z^4 - 2y^4z^4 - 2y^3z^4 - x^2z^6 - 2x^2z^5 + 4xyz^5 - 2y^2z^5 + 2xyz^6 \\
& - y^2z^6 = 0. \tag{4.12}
\end{aligned}$$

Due to the complexity of the polynomial bounds, it's not clear whether they can be combined into a single inequality as in the case for the 2-tangle triples, Eq. 4.3. See Fig. 4.1, to compare the party-symmetric constraints of the negativities and the 2-tangles.

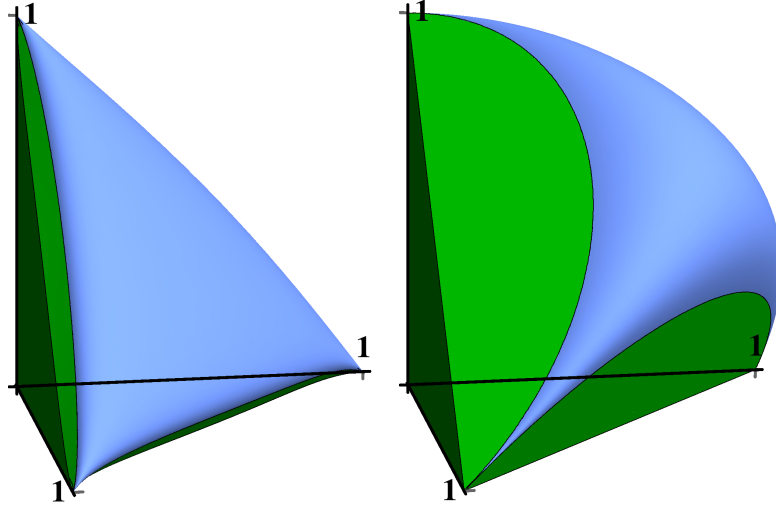


Figure 4.1: Achievable negativities (left) and 2-tangles (right), colors correspond to different polynomial bounds. For negativity, the green surface is given by Eq. 4.11 and the blue surface Eq. 4.12.

4.2 Mixed Party-Symmetric Constraints

Now we would like to talk about 3-qubit mixed states. The number of parameters it takes to describe a 3-qubit mixed state is far more than that of a pure state, so first consider an interesting special case — a mixture of a state from the W -family, $|W\rangle = a|001\rangle + b|010\rangle + c|100\rangle$, and the flipped W -family, $|\bar{W}\rangle = a'|110\rangle + b'|101\rangle + c'|011\rangle$,

$$\rho_{ABC} = \mu |W\rangle\langle W| + (1 - \mu) |\bar{W}\rangle\langle \bar{W}|, \quad (4.13)$$

with $\mu \in [0, 1]$. We will actually further remove some parameters and consider the state,

$$\rho_{ABC} = (a|001\rangle + b|010\rangle + c|100\rangle)(a\langle 001| + b\langle 010| + c\langle 100|) + d^2|011\rangle\langle 011|, \quad (4.14)$$

with $a^2 + b^2 + c^2 + d^2 = 1$, and $a, b, c, d \geq 0$. The 2-tangles are readily computed,

$$\begin{aligned}\tau_{AB} &= 2bc, \\ \tau_{AC} &= 2ac, \\ \tau_{BC} &= \text{Max}(2ab - 2cd, 0),\end{aligned}\tag{4.15}$$

and note that the convex roof 3-tangle is zero, since the W -family has zero 3-tangle. The negativities are similarly readily computed,

$$\begin{aligned}\mathcal{N}_{AB} &= -a^2 + \sqrt{a^2 + 4b^2c^2}, \\ \mathcal{N}_{AC} &= -b^2 + \sqrt{b^2 + 4a^2c^2}, \\ \mathcal{N}_{BC} &= -c^2 - d^2 + \sqrt{(c^2 - d^2)^2 + 4a^2b^2}.\end{aligned}\tag{4.16}$$

Since there are only four parameters, we can eliminate them in the same way we did for the pure negativities in the previous section. For the 2-tangles, we get a bounding surface given by the following 33-term polynomial,

$$\begin{aligned}& -x^6 + x^8 - 27x^2y^2 + 33x^4y^2 - 4x^6y^2 + 33x^2y^4 + 6x^4y^4 - y^6 - 4x^2y^6 + y^8 + 18x^3yz \\ & - 20x^5yz + 18xy^3z - 88x^3y^3z - 20xy^5z - 2x^4z^2 + 3x^6z^2 + 26x^2y^2z^2 + 29x^4y^2z^2 - 2y^4z^2 \\ & + 29x^2y^4z^2 + 3y^6z^2 + 2xyz^3 - 22x^3yz^3 - 22xy^3z^3 - x^2z^4 + 3x^4z^4 \\ & - y^2z^4 + 7x^2y^2z^4 + 3y^4z^4 - 2xyz^5 + x^2z^6 + y^2z^6 = 0.\end{aligned}$$

The negativity polynomial bound can be obtained as well and contains a lengthy 800 terms and is highly singular. See Fig. 4.2 to see how much further outside the pure state achievable sets that states of Eq. 4.13 can achieve. Note that the new achieved region is expanded for mixed states compared to pure states, already indicating that environments can enable entanglement to go beyond what is otherwise allowed.

After significant numerical tests, we can only conjecture that the above boundaries are fundamental for mixed states.

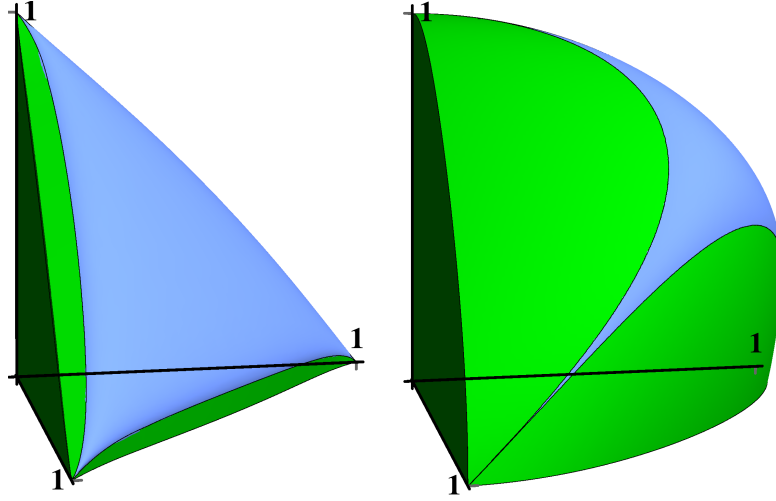


Figure 4.2: Achievable negativities (left) and 2-tangles (right) of states from Eq. 4.13, colors correspond to different polynomial bounds. For each set, the blue surface is the same as the pure state achievable set in Fig. 4.1. On the right, the green surface is given by Eq. 4.17.

4.3 Self-similarity Breeds Correlation

Regardless of whether states from Eq. 4.13 have extremal entanglement in the space of mixed states, they certainly have a lot of entanglement. In fact, they can be understood as having a purification into the 4-qubit Thue-Morse family,

$$\langle i j k l | \psi \rangle_{ABCD} = (0, \psi_{0001}, \psi_{0010}, 0, \psi_{0100}, 0, 0, \psi_{0111}, \psi_{1000}, 0, 0, \psi_{1011}, 0, \psi_{1101}, \psi_{1110}, 0), \quad (4.18)$$

with D being the auxiliary qubit. We've seen how important these states are to pure 3-qubit states (in producing the entire achievable negativity domain above), so it's no surprise that they could be important for 4-qubit states and their significance may be understood in the following sense.

First, consider that the Kronecker tensor product can very naturally lead to self-

similar fractal structures, for example, the Kronecker powers of either,

$$\rho_{\Delta} = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}, \quad \rho_{\square} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 1 \end{pmatrix},$$

immediately gives familiar shapes bearing Sierpinski's name, see Fig 4.3.

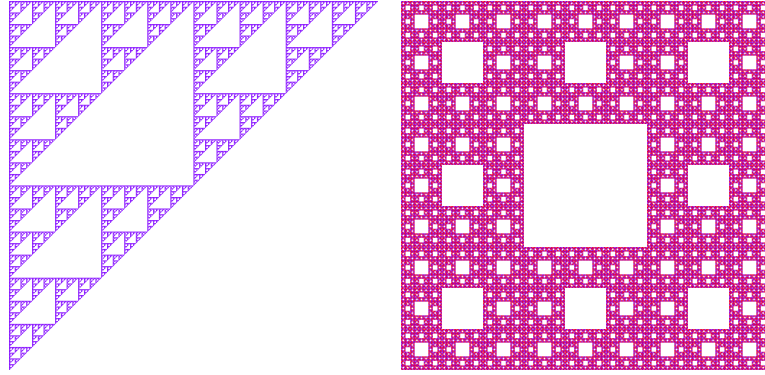


Figure 4.3: Array plots, where non-zero elements of the matrix are colored. On the left is $\rho_{\Delta}^{\otimes 8}$, and on the right is $\rho_{\square}^{\otimes 5}$.

It turns out that the Thue-Morse sequence is also an example of a Kronecker fractal, for consider the Kronecker power of the row matrix,

$$\begin{aligned} & |\text{Im}((1, i)^{\otimes n})| \\ &= (0, 1, 1, 0, 1, 0, 0, 1, 1, 0, 0, 1, 0, 1, 1, 0, 1, 0, 0, 1, 0, 1, 1, 0, 0, 1, 1, 0, 1, 0, 0, 1, \dots), \end{aligned} \tag{4.19}$$

where $|\text{Im}(\cdot)|$ means take the element-wise magnitude of the imaginary part, which then gives exactly the Thue-Morse sequence. To see visually that the sequence has self-similar properties [74], consider the turtle graphic, where the sequence is fed to a paintbrush that draws a unit line segment starting in some fixed direction if it receives a one, and then changes the direction by an angle of $\pi/3$ if it receives a zero, see Fig. 4.4.

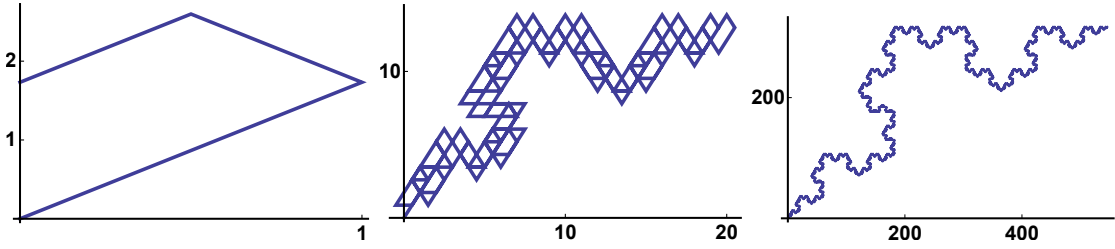


Figure 4.4: Koch snowflake emerging from the turtle graphics of the first 2^3 , 2^9 , and 2^{15} digits respectively of the Thue-Morse sequence.

It seems to then make sense to say, if the wavefunction has self-similarity properties, then the subsystems which comprise it could be highly correlated, and this is consistent with the results of this chapter.

Chapter 4, in part, is currently being prepared for submission for publication of the material as, G. W. Allen, O. Bucicovschi, and D. A. Meyer, “Another Comparison of Entanglement Measures Negativity and Concurrence.” The dissertation author is a primary investigator and author of this paper.

Chapter 5

The Dynamically Constrained: Explorations with Simple Couplings

Up until now we've been considering static properties, but importantly for physics, the wave function is compatible with theories of *change*, as long as the prescribed dynamical rule is globally unitary, for example, Schrödinger evolution. How the physical or structural properties of the wave function change depends exclusively on the specified dynamic rule. In some cases, namely entanglement, it is known how the properties change under fairly general grounds — entanglement measures, which quantify entanglement, do not increase on average under local operations and classical communication. Entanglement is often hailed as the *sine qua non* of quantum informational tasks, such as, and especially in, communication schemes. Strangely, in such contexts, even with its tendency to decay, resource counting often considers entanglement to be free [12]. It is true that the most basic of interactions can generate entangled states but it is not obvious which type or what amount lies dormant within the capabilities of the relevant system, and in this Chapter we wish to unpack some of the processes behind generating entanglement.

Using a set of polynomial entanglement measures, the tangles, we will describe all possible entanglement that can be generated from pure product states given some very basic but fundamental interactions. In this pilot study, for simplicity we will only consider, unless otherwise stated, the smallest non-trivial system of three qubits (we developed a complete description of 3-qubit entanglement in Chapter 2, which further makes for good comparisons), taking three men to task, Ising [75], Toffoli [76] and Fredkin [77], each of whom plays a critical role in physics and information theory. We find in most cases, the generated entanglement obeys a reasonably complicated polynomial inequality, and that some forms of extremal entanglement can be achieved. We then attempt to quantify the ability to generate entanglement in each process by how “bulky” the generated set is.

Coupling together product states then takes on an organic feeling that the subsystems are “growing” together as the entanglement begins to wrap them up. We thus will call the set of states generated from unentangled states the *conrescence* of the dynamics, labeled with the symbol, $\mathfrak{C}_H$, where $\mathfrak{C}$ stands for conrescence, and H will imply the couplings, for example, a certain Hamiltonian. Since we are using Fraktur to label sets, we will find occasion to talk about all of Hilbert space with the symbol $\mathfrak{H}$. Since we are really only interested in the entanglement in the conrescence, we will also use the notation $\mathfrak{C}_H(x, y, z, t)$ as the image of the conrescence in the space of $(x, y, z, t) \equiv (\tau_{A|B}, \tau_{A|C}, \tau_{B|C}, \tau_{A|B|C})$. And since t has been reserved for the 3-tangle throughout, we use the symbol χ for time, due to the Greek personification of time, Chronos ($\chi\rho\acute{o}\nu\omicron\varsigma$). Note that the idea of analyzing entanglement under dynamics here partially extends some historical work [78, 79, 80, 81, 82], but previous results focused on bipartite systems, in particular by averaging the output entanglement over input product states — so the way in which we describe our results appears to be somewhat ahistorical. In this chapter we concern ourselves only with a single application of the entangling operation, but there has also been some recent work on multiple applications [83].

5.1 Concrescence of the Ising Model

We begin this study with the weakest non-trivial couplings, given by the following Ising Hamiltonian,

$$H = \frac{1}{2} \sum_{i=0}^2 \sigma_z^{(i)} \sigma_z^{(i+1)}, \quad (5.1)$$

where exponents label the subsystem and are understood modularly with the number of sites (in this case, three). The Ising model has three local symmetries

$$[H, \sigma_z^{(j)}] = 0, \quad j = 0, 1, 2, \quad (5.2)$$

which is quite important as we are interested in the entanglement in the concrescence. We employ the above fact in the following way — since entanglement measures are invariant under local unitary matrices, we have,

$$\begin{aligned} \tau(e^{-i\chi H} |\Psi\rangle) &= \tau\left(e^{-i\theta\sigma_z^{(j)}} e^{-i\chi H} |\Psi\rangle\right) \\ &= \tau\left(e^{-i\chi H} e^{-i\theta\sigma_z^{(j)}} |\Psi\rangle\right), \end{aligned} \quad (5.3)$$

where τ stands for any entanglement measure, and therefore this shows that we can use the local symmetries to reduce the dimensionality of the set of product states with which we start. The operator $e^{-i\theta\sigma_z^{(j)}}$ induces rotations about the North pole on the Bloch sphere, which can be used to put each initial qubit onto a meridian, reducing the total number of parameters of the initial states to three. Thus, if the qubits are parametrized as $|\Psi\rangle_{ABC} = \otimes_{j=1}^3 (\cos(\theta_j/2) |0\rangle + \sin(\theta_j/2) |1\rangle)$, then after evolution, $e^{-i\chi H} |\Psi\rangle_{ABC}$, the

tangles take the following form,

$$\begin{aligned}\tau_{A|B} &= \frac{2s_1s_2\omega}{1+3\omega^2} \sqrt{1+3\omega^2-2s_3^2\omega(1+\omega)}, \\ \tau_{A|B|C} &= \frac{4s_1s_2s_3\omega^{3/2}}{1+3\omega^2},\end{aligned}\tag{5.4}$$

where $s_i = \sin(\theta_i)$ with $\theta_i \in [0, \pi]$ and $\omega = |\sin(\chi)|/\sqrt{(4-3\sin(\chi)^2)} \in [0, 1]$, where we use χ for time, and the other 2-tangles are obtained by cyclically permuting the angles. The tangles then satisfy the following algebraic relation for all time,

$$2t^4(1+3\omega^2) = ((1+\omega)t^2+2x^2) ((1+\omega)t^2+2y^2) ((1+\omega)t^2+2z^2) \tag{5.5}$$

with $(\tau_{A|B}, \tau_{A|C}, \tau_{B|C}, \tau_{A|B|C}) \equiv (x, y, z, t)$, although they do not achieve the entire corresponding hypersurface. By replacing ω with its time dependence in the tangle expressions, Eq. 5.4, a straightforward computation shows that all 2-tangles are extremized at a time of $\chi = \pi/2$, or $\omega = 1$, with negative second derivatives. At this time the tangles satisfy a simpler relation

$$p \equiv t^4 - (t^2+x^2)(t^2+y^2)(t^2+z^2) = 0, \tag{5.6}$$

a hypersurface which *can* be achieved in entirety, for the inverse is,

$$s_1 = \frac{t}{\sqrt{t^2+z^2}}, \quad s_1 = \frac{t}{\sqrt{t^2+z^2}}, \quad s_1 = \frac{t}{\sqrt{t^2+z^2}}. \tag{5.7}$$

We can project out the t variable to find constraints on (x, y, z) . Consider the map $(x, y, z, t) \mapsto (x, y, z, p)$, the volume element is proportional to the Jacobian $J = \frac{\partial(x, y, z, p)}{\partial(x, y, z, t)} = \partial_t p$, which must vanish on the non-trivial boundary of the image (as explained in Chapter 1). By then imposing the constraint $p = 0$, we look for the condition for simultaneous ze-

ros of two polynomials $(p, \partial_t p)$, which is determined by the vanishing of the discriminant, Δ , of p with respect to t , and we extract the non-trivial factor from the discriminant,

$$\begin{aligned}
\Delta_t(p) = & z^8(x-y)^2(x+y)^2 \\
& - 2z^6(x^4 + x^6 - 4x^2y^2 - x^4y^2 + y^4 - x^2y^4 + y^6) \\
& + z^4(x^4 - 2x^6 + x^8 - 10x^2y^2 - 4x^4y^2 + 2x^6y^2 + y^4 \\
& \quad - 4x^2y^4 - 6x^4y^4 - 2y^6 + 2x^2y^6 + y^8) \\
& - 2z^2x^2y^2(-2 + 5x^2 - 4x^4 + x^6 + 5y^2 + 2x^2y^2 \\
& \quad - x^4y^2 - 4y^4 - x^2y^4 + y^6) \\
& + x^4y^4(1-x+y)(1+x-y)(1-x-y)(1+x+y).
\end{aligned} \tag{5.8}$$

We would like to show explicit achievability of the region enclosed by the surface $\Delta_t(p) = 0$. For $\omega = 1$, the 2-tangles look like $(x^2, y^2, z^2) = (s_1^2 s_2^2 (1-s_3^2), s_1^2 (1-s_2^2) s_3^2, (1-s_1^2) s_2^2 s_3^2)$ and we will restrict to $\theta_i \in [0, \pi/2]$ to avoid obvious over-counting, but consider that the map may still be many-to-one, so we check for multiple solutions to $(x^2, y^2, z^2) = (\bar{x}^2, \bar{y}^2, \bar{z}^2)$ in terms of the parameters. A Gröbner calculation can eliminate all variables except, say, $(\bar{s}_1, s_1, s_2, s_3)$, which gives (besides the trivial solution $s_1 = \bar{s}_1$),

$$(1-s_1^2)\bar{s}_1^4 - (1-2s_1^2 + s_1^2 s_2^2 + s_1^2 s_3^2 - s_2^2 s_3^2)\bar{s}_1^2 - s_1^2(1-s_2^2)(1-s_3^2) = 0. \tag{5.9}$$

Based off the signs of the coefficients to $\bar{s}_1$, there is only one positive solution, and by solving the quadratic equation, the condition of $\bar{s}_1 \leq 1$ is equivalent to $4(1-s_1^2)^2 s_2^2 s_3^2 \geq 0$ and therefore the map $(s_1, s_2, s_3) \mapsto (x, y, z)$ is two-to-one. To show achievability, we ask if the volume of the parametrically described region, and the region enclosed by $\Delta_t(p) = 0$ are the same up to a factor of two.

First we compute the semi-algebraic volume $\int_{\Delta_t(p) \geq 0} dx dy dz$. A bijective bound-

ary parametrization is,

$$(x, y, z) = \left(s_1 s_2 \sqrt{s_1^2 + s_2^2 - 1}, s_2 \sqrt{1 - s_1^2} \sqrt{2 - s_1^2 - s_2^2}, s_1 \sqrt{1 - s_2^2} \sqrt{2 - s_1^2 - s_2^2} \right), \quad (5.10)$$

where (s_1, s_2) take values in $[0, 1]^2$ such that $s_1^2 + s_2^2 \geq 1$. To confirm bijectivity, the one-to-one property can be seen by computing a Gröbner basis of polynomials $(x^2 - \bar{x}^2, y^2 - \bar{y}^2, z^2 - \bar{z}^2)$ in terms of the parameters. By eliminating $(s_2, \bar{s}_2)$ with the Groöbner basis calculation, we obtain,

$$(s_1^2 - \bar{s}_1^2)^3 (s_1^2 + \bar{s}_1^2 - 2) = 0, \quad (5.11)$$

which only has one solution for $\bar{s}_1$ in the proper domain. The onto property only needs to be checked for $y + z < 1$, which is the projection of the surface onto the (y, z) plane, from where the onto property should be fairly easy to see from the parametrization by checking the boundary of the domain.

Thus the semi-algebraic volume can come from Gauss's law,

$$\begin{aligned} V &= \int_{\Delta_t(p) \geq 0} dV \\ &= \int_{\Delta_t(p) \geq 0} dV \frac{1}{3} \nabla \cdot (x, y, z) \\ &= \frac{1}{3} \int_{\Delta_t(p)=0} d\vec{A} \cdot (x, y, z) \\ &= \frac{1}{3} \int_0^1 ds_1 \int_{\sqrt{1-s_1^2}}^1 ds_2 \frac{-2s_1 s_2 (-1 + s_1^2 - s_1 s_2 + s_2^2) (-1 + s_1^2 + s_1 s_2 + s_2^2)}{\sqrt{(1-s_1^2)(1-s_2^2)(s_1^2 + s_2^2 - 1)}} \\ &= \pi/15. \end{aligned} \quad (5.12)$$

The other, parametrized volume, with parametrization,

$$(x, y, z) = (s_1 s_2 \sqrt{1 - s_3^2}, s_1 \sqrt{1 - s_2^2} s_3, \sqrt{1 - s_1^2} s_2 s_3), \quad (5.13)$$

is obtained from the integral,

$$\begin{aligned}
V &= \int_{[0,1]^3} ds_1 ds_2 ds_3 \left| \frac{\partial(x,y,z)}{\partial(s_1,s_2,s_3)} \right| \\
&= \int_{[0,1]^3} ds_1 ds_2 ds_3 \left| \frac{s_1^3 s_2 s_3 + s_1 s_2^3 s_3 + s_1 s_2 s_3^3 - 2s_1 s_2 s_3}{\sqrt{1-s_1^2} \sqrt{1-s_2^2} \sqrt{1-s_3^2}} \right| \\
&= \int_0^1 ds_1 \int_0^{\sqrt{1-s_1^2}} ds_2 \int_0^1 ds_3 \frac{-(s_1^3 s_2 s_3 + s_1 s_2^3 s_3 + s_1 s_2 s_3^3 - 2s_1 s_2 s_3)}{\sqrt{1-s_1^2} \sqrt{1-s_2^2} \sqrt{1-s_3^2}} \\
&\quad + \int_0^1 ds_1 \int_{\sqrt{1-s_1^2}}^1 ds_2 \int_0^{\sqrt{2-s_1^2-s_2^2}} ds_3 \frac{-(s_1^3 s_2 s_3 + s_1 s_2^3 s_3 + s_1 s_2 s_3^3 - 2s_1 s_2 s_3)}{\sqrt{1-s_1^2} \sqrt{1-s_2^2} \sqrt{1-s_3^2}} \\
&\quad + \int_0^1 ds_1 \int_{\sqrt{1-s_1^2}}^1 ds_2 \int_{\sqrt{2-s_1^2-s_2^2}}^1 ds_3 \frac{+(s_1^3 s_2 s_3 + s_1 s_2^3 s_3 + s_1 s_2 s_3^3 - 2s_1 s_2 s_3)}{\sqrt{1-s_1^2} \sqrt{1-s_2^2} \sqrt{1-s_3^2}} \\
&= 2\pi/15.
\end{aligned} \tag{5.14}$$

Note that the integration limits can be easily obtained via the cylindrical decomposition. So indeed, we compute $\frac{1}{2} \int_{[0,1]^3} ds_1 ds_2 ds_3 \left| \frac{\partial(x,y,z)}{\partial(s_1,s_2,s_3)} \right| = \int_{\Delta_t(p) \geq 0} dx dy dz$.

Now to be safe, we will check for a measure zero set that possibly was missed by the integration. Consider solving for the inverse map of the volume parametrization — finding the Gröbner basis of polynomials, $(x^2 - x^2(s_1, s_2, s_3), y^2 - y^2(s_1, s_2, s_3), z^2 - z^2(s_1, s_2, s_3))$ from Eq. 5.13, eliminating say, (s_2, s_3) , gives,

$$x^2 y^2 + (-2x^2 y^2 + x^2 z^2 + y^2 z^2) s_1^2 + (x^2 y^2 - z^2 - x^2 z^2 - y^2 z^2 + z^4) s_1^4 + z^2 s_1^6 = 0, \tag{5.15}$$

which is cubic in s_1^2 . Recall that the roots of a polynomial depends *continuously* on the coefficients in $\mathbb{C}$. On the other hand, the discriminant of the above polynomial in the variable s_1^2 recovers Eq. 5.8, thus with coefficients in the corresponding semi-algebraic set gives real solutions to s_1^2 , since a positive discriminant of a cubic implies all of the roots are real. Now we employ some basic point-set topology. Recall that for a

continuous function, the pre-images of closed sets are closed sets. Since the above inverse is continuous, the original parametrization, Eq. 5.13 maps the domain (closed), to a closed set. The complement of a closed set is an open set and all non-empty open sets have positive measure, therefore the complement to the image must be the empty set since there's no slack in the volume, and the following theorem is proved.

Theorem: *Every pure 3-qubit state $|\Psi\rangle_{ABC}$, that evolves from a pure product state through Ising interactions 5.1, has pairwise 2-tangles, $(\tau_{A|B}, \tau_{A|C}, \tau_{B|C}) \equiv (x, y, z)$ that satisfy, $\Delta_t(p) \geq 0$ with $\Delta_t(p)$ defined in Eq. 5.8. Conversely, for any non-negative triple (x, y, z) satisfying the inequality, there exists a pure 3-qubit product state that can evolve to a state with corresponding tangles.*

See Fig. 5.1 for a visual of the Ising concrescence.

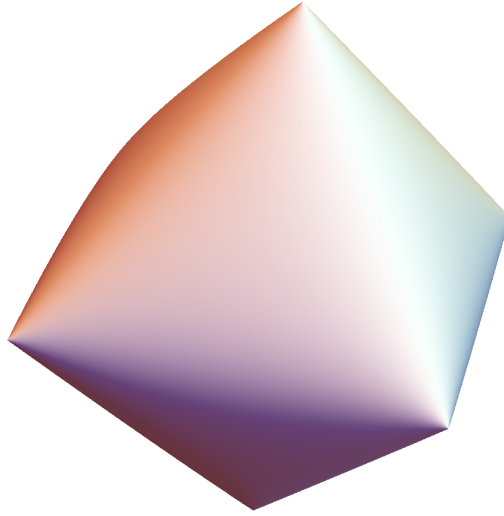


Figure 5.1: Ising concrescence is the non-negative subset of the pictured semi-algebraic set.

The Ising model still has a few more tricks up its sleeve. Consider the non-uniform coupling Ising model,

$$H = \sum_{i=0}^2 J_{i,i+1} \sigma_z^{(i)} \sigma_z^{(i+1)}, \quad (5.16)$$

with non-zero $J_{i,j} \in \mathbb{R} \setminus \{0\}$. Each of the local Hamiltonians commute,

$$[\sigma_z^{(i)} \sigma_z^{(j)}, \sigma_z^{(i')} \sigma_z^{(j')}] = 0, \quad (5.17)$$

so the evolution operator factors,

$$e^{-i\chi H} = \prod_{i,j} e^{-i\chi J_{i,j} \sigma_z^{(i)} \sigma_z^{(j)}}, \quad (5.18)$$

and each individual factor is periodic in time. If one can wait long enough in time, it is possible to approximate to arbitrary accuracy the action of the uniform coupling Ising model where the tangles were maximized from before. Hence the non-uniform coupling Ising model can achieve the same concrescence as the uniform coupling Ising model. Furthermore, since the 3-dimensional Ising concrescence, $\mathfrak{C}_{\text{Ising}}(x, y, z)$, happens to be the convex hull of itself with its coordinate plane projections, the concrescence does not change if one evolves from pure product states or mixed separable states.

The above commutation relations might be further used to say something about the Ising concrescence of arbitrarily many qubits in an arbitrary coupled Hamiltonian,

$$H = \sum_{i,j} J_{i,j} \sigma_z^{(i)} \sigma_z^{(j)}. \quad (5.19)$$

Consider when $J_{i,j} = 0$ for some i, j , in all specific cases we've checked, the 2-tangle between i, j remains zero in the concrescence for all time. In a future sequel of this work, we plan to give a general argument for why, or to what extent, this peculiar property holds.

5.2 Bell Waves in Heisenberg Model

As important as it is to identify where product states can evolve to, it should also be important to know where an entangled state evolves to. Here we'd like to report some interesting cases. Consider the nearest neighbor Heisenberg model on a ring with N sites,

$$H = \sum_{i=0}^{N-1} \vec{S}^{(i)} \cdot \vec{S}^{(i+1)}, \quad (5.20)$$

where the exponents label the tensor factor on which the operator acts and are to be understood as modulo N , and $\vec{S} = \frac{1}{2}(\sigma_x, \sigma_y, \sigma_z)$.

First we will discuss a ring of three qubits. In that case, the distinct eigenvalues of H are $\epsilon = \pm \frac{3}{4}$, so the evolution is periodic with period $T = 2\pi/|\epsilon|$, and thus time should parametrize a closed curve in the space of 2-tangles. Using the following initial condition,

$$|\psi_0\rangle = \frac{1}{\sqrt{2}} \left(|001\rangle + e^{i\pi/3} |010\rangle \right), \quad (5.21)$$

which is local-unitarily equivalent to a Bell state between B and C , we find that the evolved state is,

$$\begin{aligned} |\psi(\chi)\rangle &= e^{-i\chi H} |\psi_0\rangle \\ &= \sqrt{\frac{2}{3}} \left(\cos\left(\frac{3\chi}{4} - \frac{\pi}{6}\right) |001\rangle + e^{i\pi/3} \cos\left(\frac{3\chi}{4} + \frac{\pi}{6}\right) |010\rangle + e^{-i\pi/3} \sin\left(\frac{3\chi}{4}\right) |100\rangle \right), \end{aligned} \quad (5.22)$$

where we will again use the symbol χ for time. The above state takes the form of a W -class state, $|\psi\rangle = a|001\rangle + b|010\rangle + c|100\rangle$, which has 2-tangles of the form $(\tau_{A|B}, \tau_{A|C}, \tau_{B|C}) = (x, y, z) = 2(|bc|, |ac|, |bc|)$. The W -class 2-tangles can be readily seen to satisfy the Steiner polynomial, $x^2y^2 + x^2z^2 + y^2z^2 - 2xyz = 0$, (and the 3-tangle vanishes for all χ). Since $e^{-i\frac{T}{2}H} = -I$ and global phases are meaningless, the period is

effectively $T/2$. Notice what happens at thirds of the effective period,

$$\begin{aligned} |\psi(T/6)\rangle &= \frac{1}{\sqrt{2}} \left(e^{-i2\pi/3} |010\rangle + e^{-i\pi/3} |100\rangle \right), \\ |\psi(2T/6)\rangle &= \frac{1}{\sqrt{2}} \left(e^{i2\pi/3} |100\rangle + e^{-i\pi} |001\rangle \right). \end{aligned} \quad (5.23)$$

The Bell state is essentially hopping between pairs, for which we may as well call this phenomenon a Bell wave, see Fig. 5.2 for the evolution curve in the space of 2-tangles.

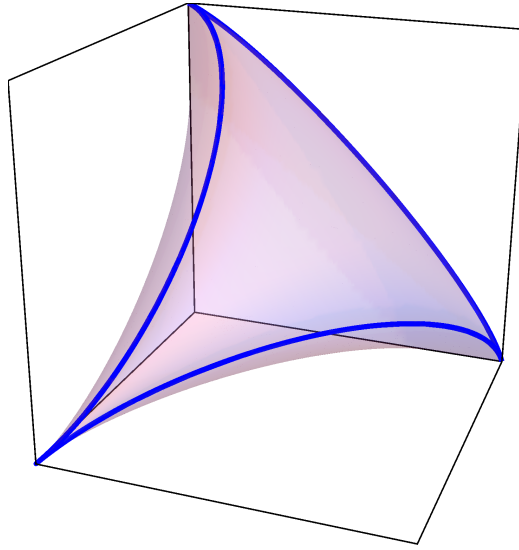


Figure 5.2: In slightly transparent purple, the positive Steiner surface lobe, and in blue, the 2-tangle evolution curve of state Eq. 5.22.

Now let's consider a four-qubit ring. The distinct eigenvalues of H are $\varepsilon = 0, \pm 1, 2$, so that the period is $T = 2\pi$. Now we use the following initial condition,

$$|\Psi_0\rangle = \frac{1}{\sqrt{2}} \left(|0001\rangle + e^{i\pi/2} |0010\rangle \right), \quad (5.24)$$

which is evolved to,

$$\begin{aligned}
 |\Psi(\chi)\rangle &= e^{-i\chi H} |\Psi_0\rangle \\
 &= \cos\left(\frac{\chi}{2}\right) \sin\left(\frac{\chi}{2} + \frac{\pi}{4}\right) |0001\rangle + e^{-i\pi/2} \cos\left(\frac{\chi}{2}\right) \sin\left(\frac{\chi}{2} - \frac{\pi}{4}\right) |0010\rangle \\
 &\quad + e^{i2\pi/2} \sin\left(\frac{\chi}{2}\right) \sin\left(\frac{\chi}{2} - \frac{\pi}{4}\right) |0100\rangle + e^{-i\pi/2} \sin\left(\frac{\chi}{2}\right) \sin\left(\frac{\chi}{2} + \frac{\pi}{4}\right) |1000\rangle.
 \end{aligned} \tag{5.25}$$

Now we look at fourths of the period,

$$\begin{aligned}
 |\Psi(T/4)\rangle &= \frac{1}{\sqrt{2}} \left(e^{-i\pi/2} |1000\rangle + |0001\rangle \right), \\
 |\Psi(2T/4)\rangle &= \frac{1}{\sqrt{2}} \left(e^{i\pi} |0100\rangle + e^{-i\pi/2} |1000\rangle \right), \\
 |\Psi(3T/4)\rangle &= \frac{1}{\sqrt{2}} \left(e^{i\pi/2} |0010\rangle + e^{i\pi} |0100\rangle \right),
 \end{aligned} \tag{5.26}$$

so that we again have a type of Bell wave. Since it is harder to visual the evolution curve in the now $\binom{4}{2} = 6$ -dimensional space of 2-tangles, we will use a graph representation. See Fig. 5.3 for the color coding we will use in the graphs, and see Fig. 5.4 for a several time snapshots of the tangles in the ring, where the vertices represent each qubit, and the edges represent the 2-tangles and the color represents the value of the 2-tangle.

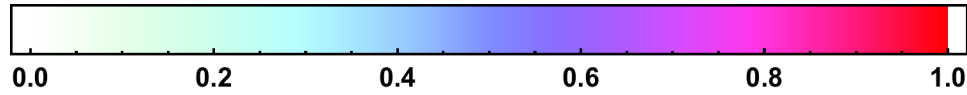


Figure 5.3: Color codes for the 2-tangle $\in [0, 1]$ in the graphs.

There is still another type of Bell wave possible in the four-qubit ring. Consider now a different initial condition given by,

$$|\Psi_0\rangle = \frac{1}{2}(|01\rangle - |10\rangle)_{AB}(|01\rangle - |10\rangle)_{CD}, \tag{5.27}$$

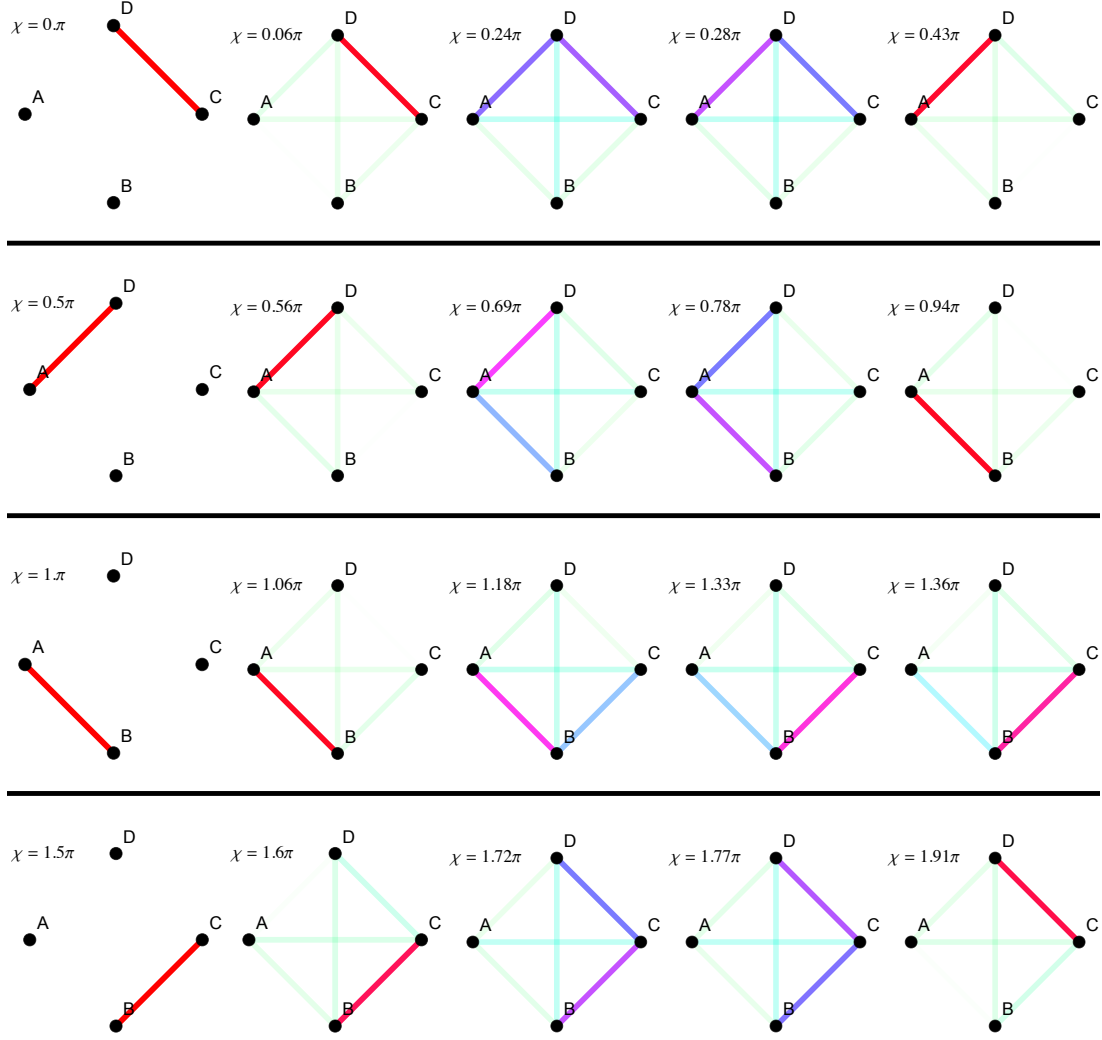


Figure 5.4: Irregular snap shots of the Bell wave around the ring.

which evolves to the following,

$$\begin{aligned}
 |\psi(\chi)\rangle = \frac{1}{2} & (e^{-i\pi/2} \sin(\chi) |0011\rangle + e^{i\chi} |0101\rangle - \cos(\chi) |0110\rangle \\
 & - \cos(\chi) |1001\rangle + e^{i\chi} |1010\rangle + e^{-i\pi/2} \sin(\chi) |1100\rangle).
 \end{aligned} \tag{5.28}$$

At a fourth of a period, the state becomes,

$$|\psi(T/4)\rangle_{ABCD} = \frac{1}{2} (|01\rangle - |10\rangle)_{AC} (|01\rangle - |10\rangle)_{BD}, \tag{5.29}$$

which returns to the initial condition at the half period, and thus we have something like two Bell waves chasing each other.

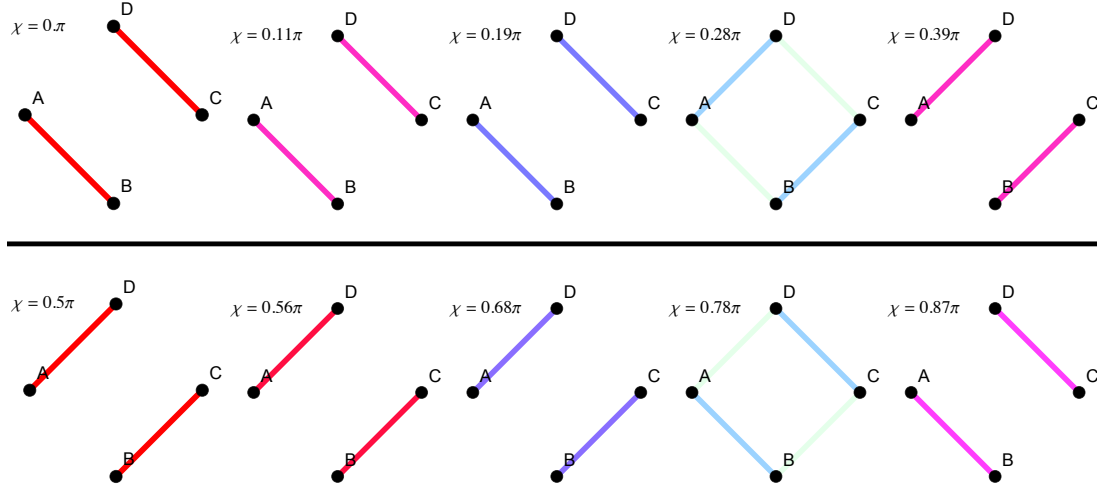


Figure 5.5: Irregular snap shots of the Bell wave around the ring.

For $N = 5$ sites, in the Hamming weight one computational basis subspace, the energies of the Hamiltonian are $\epsilon = \frac{5}{4}, \pm \frac{\sqrt{5}}{4}$, so the evolution will *not* be periodic and the entanglement is dispersed in complicated ways. Thus, the above wavelike phenomena do not seem to trivially generalize. Entanglement transfer and propagation appears to have been studied before [84], which is related to quantum state transfer *e.g.*, along a spin chain, in particular a 2-qubit state transfer [85]. Of course, teleportation [86] and entanglement swapping [87] can achieve similar displacements of states and entanglement.

5.3 Concrescence of the Toffoli Gate

Moving onto the Toffoli gate, also known as a controlled-controlled-NOT gate. In the computational basis, it is given as, $G_{\text{Toffoli}} = I_6 \oplus \sigma_x$. The gate has three local symmetries,

$$[G, \sigma_z^{(1)}] = [G, \sigma_z^{(2)}] = [G, \sigma_x^{(3)}] = 0, \quad (5.30)$$

wherefore we need only consider two qubits on a meridian, and one qubit on the (half) equator, parametrized as $|\psi\rangle_{ABC} = \frac{1}{\sqrt{2}} \begin{pmatrix} \cos(\theta_1/2) \\ \sin(\theta_1/2) \end{pmatrix} \otimes \begin{pmatrix} \cos(\theta_2/2) \\ \sin(\theta_2/2) \end{pmatrix} \otimes \begin{pmatrix} 1 \\ e^{i\theta_3} \end{pmatrix}$ with $\theta_i \in [0, \pi]$. The tangles are found to be,

$$\begin{aligned} \tau_{A|B} &= \frac{1}{2} \sqrt{1-c_1^2} \sqrt{1-c_2^2} (1-c_3), \\ \tau_{A|B|C} &= \frac{1}{2} \sqrt{1-c_1^2} \sqrt{1-c_2^2} \sqrt{1-c_3^2}, \end{aligned} \quad (5.31)$$

and the other 2-tangles are obtained by cyclically permuting the angles, which then satisfy a similar looking polynomial as before (Eq. 5.6),

$$p \equiv 4t^2xyz - (t^2 + x^2)(t^2 + y^2)(t^2 + z^2) = 0, \quad (5.32)$$

with $(\tau_{A|B}, \tau_{A|C}, \tau_{B|C}, \tau_{A|B|C}) \equiv (x, y, z, t)$. A Gröbner calculation easily shows the map $(c_1, c_2, c_3) \mapsto (x, y, z, t)$ is bijective onto the hypersurface, with inverse,

$$c_1 = \frac{t^2 - x^2}{t^2 + x^2}, \quad c_2 = \frac{t^2 - y^2}{t^2 + y^2}, \quad c_3 = \frac{t^2 - z^2}{t^2 + z^2}. \quad (5.33)$$

For a fixed, (x, y, z) how many positive solutions to t can there be? In the polynomial, p , all of the coefficients to t are obviously non-positive, except possibly the coefficient to t^2 , which *must* be positive by Decartes' rule of signs since we know at least one positive solution to t exists. Therefore the following inequality must hold

$$\frac{1}{2} \partial_t^2 p|_{t=0} = 4xyz - x^2y^2 - x^2z^2 - y^2z^2 \geq 0. \quad (5.34)$$

Descartes' rule of signs actually then guarantees two positive solutions exist, and therefore the map $(c_1, c_2, c_3) \mapsto (x, y, z)$ is two-to-one. The discriminant of p has the non-trivial

factor,

$$\begin{aligned}
\Delta_t(p) = & z^8(x-y)^2(x+y)^2 - 8z^7xy(x^2+y^2) \\
& - 2z^6(x^6 - x^4y^2 - 8x^2y^2 - x^2y^4 + y^6) \\
& + 16z^5xy(2x^4 - x^2y^2 + 2y^4) + z^4(x^8 + 2x^6y^2 \\
& - 160x^4y^2 - 6x^4y^4 - 160x^2y^4 + 2x^2y^6 + y^8) \\
& - 8z^3xy(x^6 + 2x^4y^2 - 32x^2y^2 + 2x^2y^4 + y^6) \\
& - 2z^2x^2y^2(x^6 - x^4y^2 - 8(x^4 - 10x^2y^2 + y^2) - x^2y^4 + y^6) \\
& - 8zx^3y^3(x^4 - 4x^2y^2 + y^4) + x^4y^4(x-y)^2(x+y)^2.
\end{aligned} \tag{5.35}$$

Again we check if the volume of the parametric region is twice the semi-algebraic region.

We first will want to parametrize the boundary, which was determined from the vanishing discriminant of p . A discriminant vanishes if and only if a root is degenerate. The polynomial p is cubic in t^2 and we know it has generally has two positive roots, a positive root and a negative root won't coincide, because otherwise the polynomial would take on a fairly trivial form, so then the two positive roots must coincide. This means that the parametrization of the boundary surface is bijective. If we plug in the parametrization, Eq. 5.31, into Eq. 5.35, we get two non-trivial factors,

$$\begin{aligned}
& (1 + c_1 + c_2 + c_3) \\
& \times (5 + c_1^2c_2^2 + c_2^2c_3^2 + c_1^2c_3^2 + 4c_1 + 4c_2 + 4c_3 + 2c_1c_2 + 2c_1c_3 + 2c_2c_3 \\
& - 4c_1c_2c_3 - 2c_1^2c_2c_3 - 2c_1c_2^2c_3 - 2c_1c_2c_3^2) = 0.
\end{aligned} \tag{5.36}$$

The second factor could be, say, minimized with basic calculus techniques, and happens to have local minima only on the boundary of the domain, which evaluates the polynomial to zero. And checking along the entire boundary by setting a single $c_i = \pm 1$, one can factor the polynomial into a perfect square. Therefore the polynomial is non-negative on

the boundary of the domain, and has no interior local minima so we need not consider its zeros. The other factor in the above equation has its zeros well within the domain, and these are the points mapped onto the boundary of the tangles. One can eliminate c_3 from the parametrization now,

$$\begin{aligned} x(c_1, c_2) &= \frac{1}{2}(1 + c_1 + c_2)\sqrt{(1 - c_1^2)(1 - c_2^2)}, \\ y(c_1, c_2) &= \frac{1}{2}(1 - c_2)\sqrt{-(1 - c_1^2)(c_1 + c_2)(2 + c_1 + c_2)}, \\ z(c_1, c_2) &= \frac{1}{2}(1 - c_1)\sqrt{-(1 - c_2^2)(c_1 + c_2)(2 + c_1 + c_2)}, \end{aligned} \quad (5.37)$$

and $(c_1, c_2) \in [-1, 1]^2$ such that $c_1 + c_2 \leq 0$. Applying Gauss's law again for the volume,

$$\begin{aligned} V &= \int_{\Delta_t(p) \geq 0 \wedge \partial_t^2 p|_{t=0} \geq 0} dV \\ &= \int_{\Delta_t(p) \geq 0 \wedge \partial_t^2 p|_{t=0} \geq 0} dV \frac{1}{3} \nabla \cdot (x, y, z) \\ &= \frac{1}{3} \int_{\Delta_t(p)=0 \wedge \partial_t^2 p|_{t=0} \geq 0} d\vec{A} \cdot (x, y, z) \\ &= \frac{1}{12} \int_{-1}^1 dc_1 \int_{-1}^{-c_1} dc_2 (1 - c_1)(1 - c_2)(2 + c_1 + c_2)(1 - c_1^2 - c_2^2 - c_1 - c_2 - c_1 c_2) \\ &= \frac{1}{3} \left(\frac{104}{105} \right). \end{aligned} \quad (5.38)$$

Now the parametrized volume,

$$\begin{aligned}
V &= \int_{[-1,1]^3} dc_1 dc_2 dc_3 \left| \frac{\partial(x,y,z)}{\partial(c_1,c_2,c_3)} \right| \\
&= \frac{1}{8} \int_{[-1,1]^3} dc_1 dc_2 dc_3 |(1-c_1)(1-c_2)(1-c_3)(1+c_1+c_2+c_3)| \\
&= \frac{1}{8} \int_{-1}^1 dc_1 \int_{-1}^{-c_1} dc_2 \int_{-1-c_1-c_2}^1 dc_3 (1-c_1)(1-c_2)(1-c_3)(1+c_1+c_2+c_3) \\
&\quad + \frac{1}{8} \int_{-1}^1 dc_1 \int_{-c_1}^1 dc_2 \int_{-1}^1 dc_3 (1-c_1)(1-c_2)(1-c_3)(1+c_1+c_2+c_3) \\
&\quad - \frac{1}{8} \int_{-1}^1 dc_1 \int_{-1}^{-c_1} dc_2 \int_{-1}^{-1-c_1-c_2} dc_3 (1-c_1)(1-c_2)(1-c_3)(1+c_1+c_2+c_3) \\
&= \frac{2}{3} \left(\frac{104}{105} \right),
\end{aligned} \tag{5.39}$$

and therefore, $\frac{1}{2} \int_{[-1,1]^3} dc_1 dc_2 dc_3 \left| \frac{\partial(x,y,z)}{\partial(c_1,c_2,c_3)} \right| = \int_{\Delta_t(p) \geq 0 \wedge \partial_t^2 p|_{t=0} \geq 0} dx dy dz$, and the volumes match. Appealing to continuity again gives the following theorem.

Theorem: Every pure 3-qubit output state $|\psi\rangle_{ABC}$ from a pure product input to the Toffoli gate, $I_6 \oplus \sigma_x$, has pairwise 2-tangles, $(\tau_{A|B}, \tau_{A|C}, \tau_{B|C}) \equiv (x, y, z)$ that satisfy both $\Delta_t(p) \geq 0$ defined in Eq. 5.35 and $\partial_t^2 p|_{t=0} \geq 0$, from Eq. 5.34. Conversely, for any non-negative triple (x, y, z) satisfying the inequalities, there exists a 3-qubit pure product input state that can output corresponding tangles.

See Fig. 5.6 for a visual of the Toffoli concrescence.

It might seem strange that the Toffoli concrescence has a party exchange symmetry, but recall that the Toffoli gate can change its target qubit with local unitaries, as in the following circuit equivalence,

$$\begin{array}{c}
\text{---} [H] \text{---} \bullet \text{---} [H] \text{---} \\
\text{---} \bullet \text{---} \\
\text{---} [H] \text{---} \oplus \text{---} [H] \text{---}
\end{array} = \begin{array}{c}
\text{---} \oplus \text{---} \\
\text{---} \bullet \text{---} \\
\text{---} \bullet \text{---}
\end{array}, \tag{5.40}$$

and thus we only consider two qubits on a meridian and one Santa Claus qubit, with parametrization, $|\Psi\rangle_{ABC} = \begin{pmatrix} \cos(\theta_1/2) \\ \sin(\theta_1/2) \end{pmatrix} \otimes \begin{pmatrix} \cos(\theta_2/2) \\ \sin(\theta_2/2) \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, with $\theta_i \in [0, \pi]$. The tangles take on very simplified expressions,

$$\begin{aligned} \tau_{A|B} &= \tau_{A|C} = \frac{1}{2}s_1s_2, \\ \tau_{A|B|C} &= \frac{1}{2}s_1(1 - c_2), \end{aligned} \tag{5.43}$$

with $\tau_{B|C} = 0$. The parameter θ_1 , makes the achievable tangle domain manifestly star-shaped, and for $\theta_1 = \pi/2$, the parameter θ_2 makes a circle centered at $(\tau_{A|B}, \tau_{A|C}, \tau_{A|B|C}) = (0, 0, 1/2)$.

Theorem: *Every 3-qubit output state $|\Psi\rangle_{ABC}$ from a pure product input state to the Fredkin gate, $I_5 \oplus \sigma_x \oplus I_1$, has pairwise 2-tangles, $(\tau_{A|B}, \tau_{A|C}, \tau_{B|C}, \tau_{A|B|C}) \equiv (x, y, z, t)$ that satisfy the following (in)equalities,*

$$\begin{aligned} \left(t - \frac{1}{2}\right)^2 + \left(\frac{x+y}{2}\right)^2 &\leq \frac{1}{4}, \\ x = y, \quad z = 0. \end{aligned} \tag{5.44}$$

Conversely, for any non-negative 4-tuple (x, y, z, t) satisfying the (in)equalities, there exists an pure input 3-qubit product state that can output the corresponding tangles.

Even though the Fredkin Concrescence seems smaller than the Ising and Toffoli, it is extremal in the following sense — take the polynomial constraint on all the tangles, $t^2(1 - t^2 - x^2 - y^2 - z^2) - (x^2y^2 + x^2z^2 + y^2z^2 - 2xyz) \geq 0$, and plug in $z = 0$, and $x = y$, and it simplifies to $-(t^2 - t + x^2)(t^2 + t + x^2) \geq 0$. The 2nd factor can be dropped since it's always non-negative and the remaining factor is equivalent to Eq. 5.44.

5.5 Measuring the Entangling Power

While it is important to have a fine-grained idea of the allowed entanglements, given exactly by polynomial constraints, it is sometimes useful to decrease the resolution. We propose a simple ratio of volumes between the dynamically generated entanglement allowed by evolution, and the entanglement allowed by Hilbert space. We already have most of the volumes computed from proving the theorems above — next we need the volumes of the tangle regions allowed by Hilbert space.

Considering the 2-tangles and the 3-tangle, recall from Chapter 2, the boundary of the region, *i.e.*, solutions to, $p = t^2(1 - t^2 - x^2 - y^2 - z^2) - (x^2y^2 + x^2z^2 + y^2z^2 - 2xyz) = 0$, can be parametrized with,

$$(x, y, z, t) = \frac{1}{1 - c_1 c_2 c_3} (c_1 s_2 s_3, s_1 c_2 s_3, s_1 s_2 c_3, s_1 s_2 s_3), \quad (5.45)$$

in which case, we employ the 4-dimensional divergence theorem,

$$\begin{aligned} V &= \int_{p \geq 0} dV \\ &= \int_{p \geq 0} dV \frac{1}{4} \nabla \cdot (x, y, z, t) \\ &= \frac{1}{4} \int_{p=0} d\vec{A} \cdot (x, y, z, t) \\ &= \frac{1}{4} \int_0^{\pi/2} d\theta_1 \int_0^{\pi/2} d\theta_2 \int_0^{\pi/2} d\theta_3 \frac{\sin^2(\theta_1) \sin^2(\theta_2) \sin^2(\theta_3)}{(1 - \cos(\theta_1) \cos(\theta_2) \cos(\theta_3))^4} \\ &= \sum_{k=0}^{\infty} \binom{-4}{k} (-1)^k \left(\frac{\sqrt{\pi} \Gamma(\frac{k}{2} + \frac{1}{2})}{4 \Gamma(\frac{k}{2} + 2)} \right)^3 \\ &= \frac{\pi^3}{4^4} {}_3F_2 \left[\begin{matrix} 1/2, 1/2, 5/2 \\ 2, 2 \end{matrix}; 1 \right] + \frac{1}{3^3} {}_4F_3 \left[\begin{matrix} 1, 1, 1, 3 \\ 3/2, 5/2, 5/2 \end{matrix}; 1 \right] \\ &= \frac{1}{16} \left(\frac{\pi^4 + 12 \Gamma^8(3/4)}{24 \Gamma^4(3/4)} \right) + \frac{1}{27} {}_4F_3 \left[\begin{matrix} 1, 1, 1, 3 \\ 3/2, 5/2, 5/2 \end{matrix}; 1 \right], \end{aligned} \quad (5.46)$$

where the binomial theorem is applied to the denominator on the second line. While we

have been unsuccessful at obtaining a closed form for the hypergeometric, it may be possible as a similar function evaluates¹ ${}_4F_3\left[\begin{smallmatrix} 1 & 1 & 1 & 3/2 \\ 5/2 & 5/2 & 5/2 \end{smallmatrix}; 1\right] = \frac{27}{2}(7\zeta(3) + (3 - 2K)\pi - 12)$, where $K \approx 0.916$ is Catalan's constant.

Note that the volume of the full semi-algebraic set $\{(x, y, z, t) | t^2(1 - t^2 - x^2 - y^2 - z^2) - (x^2y^2 + x^2z^2 + y^2z^2 - 2xyz) \geq 0\}$ is given by $\frac{\pi^4 + 12\Gamma^8(3/4)}{24\Gamma^4(3/4)}$. To see this we solve for z_{top} and z_{bottom} of the boundary and integrate the difference. The discriminant of the boundary polynomial over z has the factor $(1 - t^2 - x^2 - y^2)$, and so we integrate (x, y, t) over a unit 2-ball,

$$\begin{aligned}
 V &= \int dx dy dt (z_{\text{top}} - z_{\text{bottom}}) \\
 &= \int dx dy dt \frac{\sqrt{4(t^2 + x^2)(t^2 + y^2)(1 - t^2 - x^2 - y^2)}}{x^2 + y^2 + t^2} \\
 &= 2 \int r^2 dr \sin(\theta) d\theta d\phi \sqrt{1 - r^2} \sqrt{(1 - \sin^2(\theta) \sin^2(\phi)) (1 - \sin^2(\theta) \cos^2(\phi))} \\
 &= \frac{\pi}{8} \int d\theta d\phi \sin(\theta) \sqrt{(1 - \sin^2(\theta) \sin^2(\phi)) (1 - \sin^2(\theta) \cos^2(\phi))},
 \end{aligned} \tag{5.47}$$

which is then an integral over the surface of the unit 2-sphere. We convert back to cartesian coordinates $(u, v) = (\sin \theta \cos(\phi), \sin(\theta) \sin(\phi))$ with $dudv = d\theta d\phi |\cos(\theta) \sin(\theta)|$ and

¹<https://math.stackexchange.com/questions/2123298/>

continue,

$$\begin{aligned}
 V &= \pi \int_0^1 du \int_0^{\sqrt{1-u^2}} dv \frac{\sqrt{(1-u^2)(1-v^2)}}{\sqrt{1-u^2-v^2}} \\
 &= \pi \int_0^1 du \sqrt{1-u^2} \mathbf{E}(\sqrt{1-u^2}) \\
 &= \frac{\pi}{2} \int_0^1 dk \frac{k^2}{\sqrt{1-k^2}} \mathbf{E}(k) \\
 &= \frac{\pi^2}{2} \sum_{n=0}^{\infty} \frac{\sqrt{\pi} \Gamma^2(2n+1) \Gamma(n+\frac{3}{2})}{(1-2n) 2^{4n+1} \Gamma^2(n+1) \Gamma(n+2)} \\
 &= \frac{\pi^3}{2^3} {}_3F_2 \left[\begin{matrix} -1/2, 1/2, 3/2 \\ 1, 2 \end{matrix}; 1 \right] \\
 &= \frac{\pi^4 + 12\Gamma^8(3/4)}{24\Gamma^4(3/4)},
 \end{aligned} \tag{5.48}$$

where we took advantage of the known series expansion of the complete elliptic integral of the second kind, using the convention that the argument is the modulus, *i.e.*, $\mathbf{E}(k) = \int_0^{\pi/2} d\phi \sqrt{1 - k^2 \sin^2(\phi)}$, which is not the convention used by, say, Mathematica.

Going down in dimensions to the 2-tangles only, the convex hull of the Steiner surface — the integral involves three pieces: 1) the Steiner volume, 2) the region below the Steiner until the circular intersection with the hull projected downward, 3) the region outside the hull until the circular intersection of the hull with the Steiner projected downward, see Fig. 5.7.

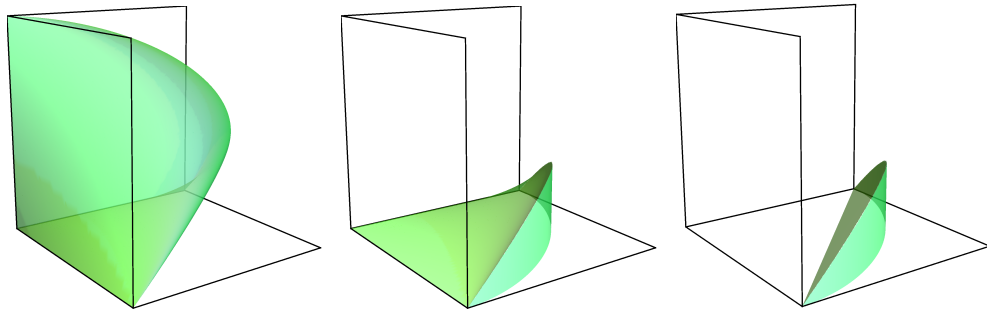


Figure 5.7: The Steiner hull broken up into three volumes for integration.

For the 1st volume, the defining equation for the Steiner surface, $x^2y^2 + x^2z^2 +$

$y^2z^2 - 2xyz = 0$, has two solutions for z , hence by going to polar,

$$\begin{aligned}
 V_1 &= \int dx \int dy (z_{\text{top}} - z_{\text{bottom}}) \\
 &= \int_0^{\pi/2} d\theta \int_0^1 dr \sqrt{1-r^2} \sin(2\theta) r \\
 &= 1/3.
 \end{aligned} \tag{5.49}$$

As a side comment, it is interesting to note how close in volume this is to the Toffoli concrescence.

The 2nd volume needs the relation between x and y at the intersection of the plane with the Steiner surface. Eliminating z from the Steiner definition and $z = x + y - 1$, gives the relation (in polar), $r(2 + \sin(2\theta)) = 2(\cos(\theta) + \sin(\theta))$. Therefore,

$$\begin{aligned}
 V_2 &= \int dx \int dy (z_{\text{bottom}}) \\
 &= \int_0^{\pi/2} d\theta \int_0^{\frac{2(\cos(\theta)+\sin(\theta))}{(2+\sin(2\theta))}} dr \sin(\theta) \cos(\theta) \left(1 - \sqrt{1-r^2}\right) r \\
 &= \frac{\pi}{27\sqrt{3}}.
 \end{aligned} \tag{5.50}$$

The 3rd volume gets cut off when $x + y = 1$, which forms the lower bound of the polar integral,

$$\begin{aligned}
 V_3 &= \int dx \int dy (z_{\text{plane}}) \\
 &= \int_0^{\pi/2} d\theta \int_{\frac{1}{\cos(\theta)+\sin(\theta)}}^{\frac{2(\cos(\theta)+\sin(\theta))}{(2+\sin(2\theta))}} dr (r \cos(\theta) + r \sin(\theta) - 1) r \\
 &= \frac{1}{6} - \frac{2\pi}{27\sqrt{3}}.
 \end{aligned} \tag{5.51}$$

Finally, by combining the volumes,

$$V = V_1 + 3(V_2 - V_3) = \frac{1}{4} \left(\frac{4\pi}{3\sqrt{3}} \right) - \frac{1}{6} \tag{5.52}$$

Note that the volume of the full semi-algebraic set, the convex hull of the Steiner surface,

$$(1 - x^2 - y^2 - z^2) + \sqrt{(1 - x - y + z)(1 - x + y - z)(1 + x - y - z)(1 + x + y + z)} \geq 0,$$

including all octants, is given by $\frac{4\pi}{3\sqrt{3}}$.

There are a few more non-trivial volumes that we will compute. The first is the 4-dimensional volume of the Ising concrescence,

$$\begin{aligned} V &= \int_{[0,1]^4} ds_1 ds_2 ds_3 d\omega \left| \frac{\partial(x, y, z, t)}{\partial(s_1, s_2, s_3, \omega)} \right| \\ &= \int_{[0,1]^4} \frac{ds_1 ds_2 ds_3 d\omega \, 32(1 + 3\omega^2)^{-2} s_1^2 s_2^2 s_3^2 (3 - s_1^2 - s_2^2 - s_3^2) \omega^{11/2}}{\sqrt{(1 + 3\omega^2 - 2s_1^2 \omega(1 + \omega))(1 + 3\omega^2 - 2s_2^2 \omega(1 + \omega))(1 + 3\omega^2 - 2s_3^2 \omega(1 + \omega))}} \\ &= \int_0^1 \frac{d\omega \, 3\sqrt{\omega}}{32\sqrt{2}(1 + 3\omega^2)^2} \left((\omega - 1)\sqrt{2\omega(1 + \omega)} + (1 + 3\omega^2) \cos^{-1}\left(\frac{1 - \omega}{\sqrt{1 + 3\omega^2}}\right) \right)^2 \\ &\quad \times \left[\frac{8\sqrt{\omega}}{(1 + \omega)^{9/2}} \left((\omega - 1)\sqrt{2\omega(1 + \omega)} + (1 + 3\omega^2) \cos^{-1}\left(\frac{1 - \omega}{\sqrt{1 + 3\omega^2}}\right) \right) \right. \\ &\quad \left. + \left(\frac{(1 - \omega)\sqrt{2\omega(1 + \omega)}(3 + 4\omega + 13\omega^2) - 3(1 + 3\omega^2)^2 \cos^{-1}\left(\frac{1 - \omega}{\sqrt{1 + 3\omega^2}}\right)}{(1 + \omega)^5 \sqrt{\omega(1 + \omega)}} \right) \right] \\ &\approx 0.0271981, \end{aligned} \tag{5.53}$$

which we can only seem to perform numerically. Recall that this 4-dimensional volume is bounded by the hypersurface given by, $p = t^4 - (t^2 + x^2)(t^2 + y^2)(t^2 + z^2) = 0$. For

comparison we compute the volume enclosed by this surface,

$$\begin{aligned}
V &= \int_{p \geq 0} dV \\
&= \int_{p \geq 0} dV \frac{1}{4} \nabla \cdot (x, y, z, t) \\
&= \frac{1}{4} \int_{p=0} d\vec{A} \cdot (x, y, z, t) \\
&= \frac{1}{4} \int_{[0,1]^3} \frac{ds_1 ds_2 ds_3 s_1^2 s_2^2 s_3^2}{\sqrt{(1-s_1^2)(1-s_2^2)(1-s_3^2)}} \\
&= \pi^3 / 4^4 \\
&\approx 0.121118.
\end{aligned} \tag{5.54}$$

Relatedly, note that the following holds about this region,

$$\begin{aligned}
0 &\leq t^4 - (t^2 + x^2)(t^2 + y^2)(t^2 + z^2) \\
&\leq t^4 - r^2(t^2 + x^2)(t^2 + y^2)(t^2 + z^2),
\end{aligned} \tag{5.55}$$

if the parameter $r \in [0, 1]$. Then also,

$$\begin{aligned}
0 &\leq r^4 (t^4 - r^2(t^2 + x^2)(t^2 + y^2)(t^2 + z^2)) \\
&\leq (rt)^4 - ((rt)^2 + (rx)^2)((rt)^2 + (ry)^2)((rt)^2 + (rz)^2),
\end{aligned} \tag{5.56}$$

meaning that $r(x, y, z, t)$ satisfies $p \geq 0$ if (x, y, z, t) does, meaning that the domain of $p \geq 0$ is star-shaped, implying that the Ising concrescence is not star-shaped (and by extension not convex) and only achieves about 22% of the volume enclosed by $p = 0$. Also the surface defined by $p = 0$ roughly cuts the full 4-dimensional achievable set in half. We will call the region bounded by $p = 0$, the star-completion of the concrescence, $\mathfrak{C}_{\text{Ising}}^{\text{Star}}(x, y, z, t)$.

In a similar vein, the Toffoli concrescence makes a hypersurface in 4-dimensions,

given by $p_{\text{Toff}} = 4t^2xyz - (t^2 + x^2)(t^2 + y^2)(t^2 + z^2) = 0$. The region enclosed by $p_{\text{Toff}} \geq 0$ is star-shaped by an analogous argument as above. The enclosed volume, *i.e.*, the star-completion, $\mathfrak{C}_{\text{Toffoli}}^{\text{Star}}(x, y, z, t)$, is,

$$\begin{aligned}
 V &= \int_{p \geq 0} dV \\
 &= \int_{p \geq 0} dV \frac{1}{4} \nabla \cdot (x, y, z, t) \\
 &= \frac{1}{4} \int_{p=0} d\vec{A} \cdot (x, y, z, t) \\
 &= \frac{1}{64} \int_{[-1,1]^3} dc_1 dc_2 dc_3 (1 - c_1)(1 - c_2)(1 - c_3) \sqrt{(1 - c_1^2)(1 - c_2^2)(1 - c_3^2)} \\
 &= \frac{1}{2} \frac{\pi^3}{4^4} \\
 &\approx 0.0605591,
 \end{aligned} \tag{5.57}$$

which is *exactly* half of the volume of the 4-dimensional star-completion of the Ising concrescence.

The last non-trivial region we will consider is the Toffoli concrescence of only party A 's 2-tangles. Projecting the Toffoli concrescence onto a coordinate plane, the boundary equation $p = (-x^6 + x^8 - 27x^2y^2 + 33x^4y^2 - 4x^6y^2 + 33x^2y^4 + 6x^4y^4 - y^6 - 4x^2y^6 + y^8) = 0$, can be parametrized as,

$$(x, y) = \left(s(1 + 2s^2)\sqrt{1 - s^2}, (1 - s^2)\sqrt{1 - 4s^2} \right), \tag{5.58}$$

where the parameter takes values $s \in [0, \frac{1}{\sqrt{2}}]$. Applying the two-dimensional Gauss's law,

$$\begin{aligned}
V &= \int_{p \leq 0} dV \\
&= \int_{p \leq 0} dV \frac{1}{2} \nabla \cdot (x, y) \\
&= \frac{1}{2} \int_{p=0} d\vec{A} \cdot (x, y) \\
&= \frac{1}{2} \int_0^{1/\sqrt{2}} ds \sqrt{\frac{(1-s^2)(1+2s^2)(1+4s^2-8s^4)^2}{1-2s^2}} \\
&= \frac{\sqrt{17}}{32\sqrt{2}} \int_0^{\pi/2} d\theta (5 - \cos(4\theta)) \sqrt{1 - \frac{1}{17} \cos(4\theta)} \\
&= \frac{\sqrt{17}\pi}{64\sqrt{2}} \sum_{n=0}^{\infty} \left(\binom{1/2}{2k} \frac{5\Gamma(k+1/2)}{17^{2k}\Gamma(k+1)} + \binom{1/2}{2k+1} \frac{\Gamma(k+3/2)}{17^{2k+1}\Gamma(k+2)} \right) \\
&= \mathbf{E}(1/3) - \frac{1}{2} \mathbf{K}(1/3),
\end{aligned} \tag{5.59}$$

where $\mathbf{K}, \mathbf{E}$ are respectively the complete elliptic integrals of the 1st and 2nd kind as functions of the elliptic modulus.

See Table 5.1 for the collection of volume calculations, recalling the notation — a Fraktur letter indicates the domain with $\mathfrak{H}$ being the full Hilbert space and $\mathfrak{C}$ being the concrescence where the subscripts indicate the specific coupling, the usual equivalence $(x, y, z, t) \equiv (\tau_{AB}, \tau_{AC}, \tau_{BC}, \tau_{ABC})$, so that $\mathfrak{C}(x, y, z, t)$ means the concrescence (as a set of evolved states) mapped in the space of tuples (x, y, z, t) , and finally a superscript Star means that the domain is the star-completion with respect to the origin.

Chapter 5, in part, is currently being prepared for submission for publication of the material as, G. W. Allen and D. A. Meyer, “Complex Entanglement Constraints under Simple Dynamics: Ising, Toffoli, and Fredkin.” The dissertation author is a primary investigator and author of this paper.

Table 5.1: Table of Volumes

Domain	Exact Volume	Approximate Volume
$\mathfrak{H}(x, y, z, t)$	$\frac{1}{16} \left(\frac{\pi^4 + 12\Gamma^8(3/4)}{24\Gamma^4(3/4)} \right) + \frac{1}{27} {}_4F_3 \left[\begin{matrix} 1 & 1 & 1 & 3 \\ 3/2 & 5/2 & 5/2 \end{matrix}; 1 \right]$	0.270
$\mathfrak{H}(x, y, z)$	$\frac{1}{4} \left(\frac{4\pi}{3\sqrt{3}} \right) - \frac{1}{6}$	0.438
$\mathfrak{H}(x, y)$	$\frac{\pi}{4}$	0.785
$\mathfrak{H}(x)$	1	1.000
$\mathfrak{C}_{\text{Ising}}^{\text{Star}}(x, y, z, t)$	$\frac{\pi^3}{4^4}$	0.121
$\mathfrak{C}_{\text{Ising}}(x, y, z, t)$	—	0.027
$\mathfrak{C}_{\text{Ising}}(x, y, z)$	$\frac{\pi}{15}$	0.209
$\mathfrak{C}_{\text{Ising}}(x, y)$	$\frac{1}{2}$	0.500
$\mathfrak{C}_{\text{Ising}}(x)$	1	1.000
$\mathfrak{C}_{\text{Toffoli}}^{\text{Star}}(x, y, z, t)$	$\frac{\pi^3}{2 \cdot 4^4}$	0.061
$\mathfrak{C}_{\text{Toffoli}}(x, y, z, t)$	0	0.000
$\mathfrak{C}_{\text{Toffoli}}(x, y, z)$	$\frac{1}{3} \left(\frac{104}{105} \right)$	0.330
$\mathfrak{C}_{\text{Toffoli}}(x, y)$	$\mathbf{E}\left(\frac{1}{3}\right) - \frac{1}{2} \mathbf{K}\left(\frac{1}{3}\right)$	0.716
$\mathfrak{C}_{\text{Toffoli}}(x)$	1	1.000
$\mathfrak{C}_{\text{Fredkin}}(x, y, z, t)$	0	0.000
$\mathfrak{C}_{\text{Fredkin}}(x, y, z)$	0	0.000
$\mathfrak{C}_{\text{Fredkin}}(x, y)$	0	0.000
$\mathfrak{C}_{\text{Fredkin}}(x)$	$\frac{1}{2}$	0.500

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