Entanglement has been long recognized as a resource for quantum informational tasks [1] and recently, entanglement has played a role in manifesting novel phases of matter [2]. In each setting, the quantitative theory of entanglement aids the analysis. An important result of quantitative theory is the strict bounds it places on the entanglement between Alice's qubit and Bob's qubit is limited by the entanglement between Alice's qubit with Charlie's. The property was first captured by concurrence in the following monogamy inequality [7],

$$C_{ABC}^2 \geq C_{AB}^2 + C_{AC}^2,$$  \hspace{1cm} (1)

where C is the concurrence, subscripts label the parties, and the vertical bar indicates the bipartite splitting with which to compute the concurrence. In this way, if $C_{ABC}^2 \approx C_{AB}^2 \approx 1$, then $C_{AC}^2 \approx 0$, hence the personification of entanglement.

To demonstrate the tightness of (1), it is informative to develop a pictorial representation. Consider the achievable set of triples, $(C_{AC}^2, C_{AB}^2, C_{ABC}^2)$, computed for all pure states of 3 qubits. The equality in (1) then defines a plane in the ambient space, $[0,1]^3$. The original work [7] 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. 1.

The elegance and simplicity of the monogamy inequality has made it the paragon for entanglement shareability. It has since been shown that entanglement of formation [8], squashed entanglement [9], and entanglement negativity [10], all satisfy the same monogamy relation.

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 [11], cannot be distilled [12]. Further, negativity provides an alternative measure of mixed state entanglement that has the extremely rare property of being computable. In this Letter, we show that the ‘linear’ monogamy inequality exemplified in (1) fails to describe the achievable set of negativity triples and we derive the true boundary. By generalizing our approach to qubits, we are then able to formulate a conjecture on the strict shareability of negativity in arbitrarily large quantum systems.

Negativity is based on the failure of the transpose operation to preserve positivity when acting on subsystems [12]. 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:

$$N_{AB} = N(\rho_{AB}) = 2 \sum_n \lambda_n^{T_A} (\rho_{AB}^T),$$  \hspace{1cm} (2)

where $\rho_{AB}^T$ 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 [13]. Negativity is sufficient to detect any entanglement in $2 \times 2$, i.e., two qubit systems [14]. Although failing to respond faithfully in general, it does bound, e.g., distillable entanglement [12] and remains widely used. One can straightforwardly verify that for pure $2 \times 2$ systems, negativity and concurrence agree, $N = C$. When extended to mixed states, due to the convexity of negativity [12], we have

$$C(\rho_{AB}) = \inf \sum_n p_n C(|\psi^{(n)}_{AB}|) = \inf \sum_n p_n N(|\psi^{(n)}_{AB}|) \geq \inf \mathcal{N} \left( \sum_n p_n |\psi^{(n)}_{AB}\rangle \langle \psi^{(n)}_{AB}| \right) = \mathcal{N}(\rho_{AB}),$$

see also [15]. Also, for pure 3-qubit states, $N_{A|BC} = C_{A|BC}$, and therefore the same monogamy inequality is satisfied,

$$N^2_{A|BC} \geq N^2_{A|B} + N^2_{A|C}, \quad (3)$$
as noted above.

In order to find the tighter monogamy inequality, i.e., the boundary of the achievable set $(N^2_{A|C}, N^2_{A|B}, N^2_{A|BC})$, 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 [16]. One such form is given as

$$|\Psi\rangle = d|000\rangle + \omega|100\rangle + a|101\rangle + b|110\rangle + c|111\rangle \quad (4)$$

with real $a, b, c, d \geq 0$, $\omega \in \mathbb{C}$, and the usual normalization. The boundary will be computed from “below” by maximizing the negativities in this parametrization.

Qubit negativity necessarily satisfies $0 \leq N \leq 1$. We find the one-two party split negativity straight forwardly,

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

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

To calculate $N^2_{A|C}$, we need the following fact: a partial transpose cannot produce more than $(D - 1)^2$ negative eigenvalues for two entangled $D$-dimensional systems [17]. Accordingly, for two-qubit states, $\rho_{AC}^{T_B}$ has no more than one negative eigenvalue. The negativity is twice the negative eigenvalue, and thus satisfies the quartic polynomial equation,

$$0 = \det[2\rho_{AC}^{T_B} + \mathcal{N}_{A|C}I_4] = -16a^4d^4 - 16a^2c^2d^4 - 8a^4d^2x + 8a^2b^2d^2x - 8a^2c^2d^2x - 8a^4d^2x + 8a^2d^2|\omega|^2x + 4a^2b^2x^2 + 4b^2d^2x^2 + 4c^2d^2x^2 + 4c^2|\omega|^2x^2 + 2a^2x^3 + 2b^2x^3 + 2c^2x^3 + 2|x|^2x^3 + x^4 - (16d^2x + 8x^2)abc|\omega| \cos(\arg(\omega)), \quad (5)$$

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

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

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 (5) with respect to $\omega$ and setting $\partial x/\partial \omega = 0$ gives

$$x(4abcd^2 + 4a^2d^2x + 4abcdx - 2c^2\omega x - \omega x^2) = 0. \quad (6)$$

The 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 (5) to maximize with respect to $c$ gives:

$$8a^2cd^4 + 4a^2d^2x + 4abcd\omega x - 2c^2d^2x^2 + 2ab\omega x^2 - 2c\omega^2x^2 - cx^3 = 0. \quad (7)$$

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 [18], will give polynomials with the proper variables eliminated. The Gröbner basis for Eqs. 5 (with $\omega \in \mathbb{R}$), 6 and 7 has a single element; setting it to zero gives:

$$(2ad - x)(2a^2 + x)(2ad + x)(2d^2 + x) \times (2a^2d^2 + a^2x - b^2x^2)(4a^2d^2 - 2b^2x - x^2) = 0. \quad (8)$$

Neglecting negative solutions for $x$ leaves three options: $x = 2ad$, and $x = -b^2 + \sqrt{b^2 + 4a^2d^2}$, 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 $x$, $\omega$, $c$, given the following constraints, $x = 2a^2d^2/(b^2 - a^2)$, Eqs. 5 (with $\omega \in \mathbb{R}$), 6, and normalization, produces,

$$a^7b^3d^4(a^2 - b^2 - ad)(a^2 - b^2 + ad)(-a^2 + b^2 + 2a^2d^2)^2 = 0, \quad (9)$$
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,

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

(10)

These triples come from precisely the condition that $\omega = c = 0$, leaving states in (4) that are locally equivalent to the $W$ class, the same class that maximize concurrence. The three components of (10) 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:

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

(11)

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 (11) 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,

$$
\begin{align*}
\det \rho_{A|C}^T &= -a^2d^4(a^2 + c^2), \\
\det \rho_{A|B}^T &= -b^2d^4(b^2 + c^2).
\end{align*}
$$

Since $\mathcal{N}_{A|BC} = 4(1 - d^2)d^2$, 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. 2 for the achievable negativity set.

The states whose negativities fill up the region shown in Fig. 2 can be understood to have a special form, which is useful for generalizing this result to higher dimensional tensor factors. From (4) with $\omega = 0$,

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

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 $|\text{GHZ}\rangle \rightarrow \sum_j |jjj\rangle$.

$$
|\Psi\rangle = d|000\rangle + \sum_{j=1}^{D-1} a|0j0\rangle + b|jj0\rangle + c|jjj\rangle.
$$

(12)

The partial transpose of the reduced density operator for (12) block diagonalizes to:

$$
\rho_{A|C}^T = \left(\begin{array}{ccc}
d^2 & 0 & ad \\
0 & a^2d^2 & 0 \\
ad & 0 & bc
\end{array}\right)
$$

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

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

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

$$
\begin{align*}
\det \rho_{A|C}^T &= (-1)^{\frac{|\mathcal{N}_{A|C}|}{2}}d^2((a^2 + c^2)d^2)^{(D-1)}a^{2(D-1)(D-2)} \\
\det \rho_{A|B}^T &= (-1)^{\frac{|\mathcal{N}_{A|B}|}{2}}d^2((b^2 + c^2)d^2)^{(D-1)}b^{2(D-1)(D-2)},
\end{align*}
$$

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 bound; however already in the \( D = 3 \) case, the polynomial is rather complicated, containing 143 terms. It is worth mentioning that naïvely testing the conjecture numerically is nearly hopeless, since the non-universality of random states are highly non-uniform throughout the achievable set [19]. Nevertheless, testing for perturbations of our boundary 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, \( C \),

\[
|\Psi\rangle = \left( d(00) + \sum_{j=1}^{D-1} b_{jj} \right) |0\rangle.
\]  

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,

\[
H_{\text{SWAP}} = \bigoplus_{j \leq k} \sigma_{x}^{(jk)},
\]

where \( \sigma_{x}^{(jk)} \) is \( \sigma_{x} \) 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 (13):

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

Then the phases can be cleaned up with local unitaries to match (12), with \( c = 0 \).

Note that the boundary states (14) produce a surface that extends and folds back into the achievable set depending on the value of \( d \), i.e., only maximizing the pairwise non-universality when \( d > 1/\sqrt{D} \), as seen from parametrically plotting the resulting polynomial surface in Fig. 3. Recall that negativity for \( D \times D \) systems has bounds \( 0 \leq \mathcal{N} \leq D - 1 \) [1].

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 [20]; for three qudits it is,

\[
\sum_{n=1}^{D-1} \lambda_{n}^{(A)} \leq \sum_{n=1}^{D-1} \lambda_{n}^{(B)} + \sum_{n=1}^{D-1} \lambda_{n}^{(C)},
\]  

including permutations of the parties, where \( \lambda_{n}^{(P)} \leq \lambda_{n+1}^{(P)} \), \( n \in \{1, \ldots, D - 1\} \) are the ascending eigenvalues of party \( P \)'s state. The marginal eigenvalues of (12) with \( c = 0 \) are

\[
\lambda^{(A)} = \{(a^2 + b^2)(D - 1), d^2\}
\]

\[
\lambda^{(B)} = \{(b^2)(D - 1), (D - 1)a^2 + d^2\}
\]

\[
\lambda^{(C)} = \{(a^2)(D - 1), (D - 1)b^2 + d^2\},
\]

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

\[
(D - 1)(a^2 + b^2) \leq (D - 1)a^2 + (D - 1)b^2.
\]

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

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

(16)

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

\[
\mathcal{N}_{A|BC} \geq \mathcal{N}_{A|B} + \mathcal{N}_{A|C},
\]

up to terms of \( O(1/D) \). See Fig. 4 for the achievable negativities without squares, \( (\mathcal{N}_{A|C}, \mathcal{N}_{A|B}, \mathcal{N}_{A|BC}) \).

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 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 qudits, provided the proper 3-qutrit canonical form is found. For arbitrary dimensions we suspect an intimate connection with marginal eigenvalue constraints...
FIG. 4: Achievable $D \to \infty$ negativity of states (12).

since our boundary states saturate the eigenvalue boundaries.

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