Pairwise Concurrence in Cyclically Symmetric Quantum States

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We provide an initial characterization of pairwise concurrence in quantum states which are invariant under cyclic permutations of party labeling. We prove that maximal entanglement can be entirely described by adjacent pairs, then give explicit descriptions of those states in specific subsets of 4 and 5 qubit states - X states. We also construct a monogamy bound on shared concurrences in the same subsets in 4 and 5 qubits, finding that above non-maximal entanglement thresholds, no other entanglements are possible.

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INTRODUCTION

Entanglement in quantum mechanics has been an exciting avenue of research in physics since its discovery. It plays a central role in quantum computing [1] [2] and offers meaningful contributions to high energy theory [3] and condensed matter physics [4] [5]. Despite the attention that entanglement has received, its fundamental properties are still not fully understood. Constraints on entanglement are generally challenging to compute due to the fact that many entanglement measures involve extremizations which are difficult to handle analytically. Those measures which do have a closed function on state parameters are difficult to calculate for high dimensional systems and many particles.

A common approach to studying these large Hilbert spaces is to consider entanglement in some smaller subspace which reduces the number of state parameters. Entanglement has been studied in states which are invariant under permutation of party labeling [6], X-states [7], and matrix product states [8] among other subsets. This paper considers the pairwise concurrence entanglement measure, defined in [9], of n qubit states which are invariant under cyclic permutation of party labeling. These cyclically symmetric (CS) states are of significant interest to translation-invariant condensed matter systems [10] [11] [12] and 1-D spin chains with periodic boundary conditions [13]. Their SLOCC properties were also examined in [14].

The CS subspace of an n qubit system offers a significant simplification to the entanglement picture by constraining the number of allowable distinct types of entanglement. Any subset or partitioning of parties to calculate entanglement among, no matter the measure of entanglement, would be equated to that of other sets of parties by the cyclic permutation invariance of the state. We narrow this picture by only examining pairwise entanglements as measured by the concurrence, \( C \), which is chosen for its relative analytic simplicity and for its relationship to the entanglement of formation [11]. The cyclic symmetry implies that for any pairwise concurrence \( C_{i,j} \) between parties \( i \) and \( j \), \( C_{i,j} = C_{i+k,j+k} \), where the party label subscripts are to be evaluated mod \( n \). So each allowable pairwise concurrence in CS-states corresponds to the spacing between party labelings. As a point of notation, define \( C^{(n)}_k \) to be the pairwise concurrence between parties \( k \)-away in an \( n \) qubit CS-state. Note that \( k \) runs from 1 to \( \lfloor \frac{n}{2} \rfloor \) as any \( k > \frac{n}{2} \) is equivalent to the \( n-k \) spacing. The \( \lfloor \frac{n}{2} \rfloor \) distinct \( C^{(n)}_k \) is reduced from the \( \binom{n}{2} \) distinct pairs in a general \( n \) qubit state.

The entanglement picture in CS-states is further simplified by the fact that many \( C^{(n)}_k \) share the same properties. To see this, consider some \( m \) which is not a factor of \( n \), and the associated permutation, \( \pi \in S_n \),

\[
\pi : i \mapsto m i \mod n.
\] (1)

Note that \( \pi \) is invertible only when \( m = 1 \) or \( m \nmid n \). Where obvious, we will interchangeably use \( \pi \) to denote the permutation on the tensor factors, as well as the associated unitary operator acting on the state. Permuting the party labels of some CS-state, \( |\psi\rangle \), according to \( \pi^{-1} \) will leave the state in some new CS-state, \( |\chi\rangle = \pi^{-1} |\psi\rangle \), which obeys \( C_{i,j} (|\psi\rangle) = C_{\pi(i),\pi(j)} (|\chi\rangle) \). This means that any properties of \( C^{(n)}_k \) will be shared by \( C^{(n)}_{m_k} \) for each \( m \) which is not a factor of \( n \). It then suffices to only examine the constraints on \( C^{(n)}_k \) for \( k \mid n \).

These simplifications, along with the natural reduction in state parameters, makes an analytic description of the CS entanglement more approachable. This paper makes a preliminary attempt at analyzing the allowed pairwise concurrences in CS-states. First, we prove that maximal entanglement in CS-states can be entirely understood in terms of the maxima of \( C^{(n)}_1 \) and explicitly determine the maxima on the X-state subspace for 4 and 5 qubits. We then discuss the bounds on multiple correlations, again with an analytic description for X-states in 4 and 5 qubits. Due to the extensive nature of the calculations, significant portions of analysis are relegated to the appendices.

MAXIMALLY ENTANLEED STATES

A natural question when examining a subset of quantum states is which states maximize entanglement within
that subset, and what is that maximal entanglement? As a result of the discussion in the previous section, we need only examine the maxima of $C_k^{(n)}$ for $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$ which are not factors of $n$. Denote a state which maximizes $C_k^{(n)}$ as $\ket{\psi_k^{(n)}}$. Finding the $\ket{\psi_k^{(n)}}$ and the associated maximal $C_k^{(n)}$ is greatly simplified by the following theorem.

**Theorem 1.** For $k|n$, $\max \{ C_k^{(n)} = \max \left( C_k^{(n)} \right) \} \text{ and a corresponding state which maximizes } C_k^{(n)}$ can be constructed as

$$\left\vert \psi_k^{(n)} \right\rangle = \bigotimes_{i=0}^{k-1} \left\vert \psi_1^{(n/k)} \right\rangle_{k(n/k)+i},$$

where $\{n/k\}$ represents the set of integers from 0 to $n/k-1$. These integers, multiplied by $k$ then incremented by $i$, indicate the party labelings in the overall state.

**Proof.** Consider some $n$ qubit CS-state, $\ket{\psi^{(n)}} = \sum_{i \in \mathbb{Z}_n^k} \psi_i \ket{i}$ and some $k|n$. Examine the reduced density matrix,

$$\rho_{k(n/k)} = \text{Tr}_{k(n/k)} \left( \left\vert \psi^{(n)} \right\rangle \left\langle \psi^{(n)} \right\vert \right)$$

$$= \sum_{j \in \mathbb{Z}_n^{n/k}} \sum_{a,b \in \mathbb{Z}_n^{n/k}} \psi_{j,a} \left\vert a \right\rangle \left\langle b \right\vert \psi_{j,b}^{*},$$

where $a$ and $b$ indicate basis elements in the parties in $k \{n/k\}$, while $j$ indicate basis elements in the remaining $n-k$ parties. Notably, this reduced state obeys, by definition,

$$C_k^{(n/k)} \left( \rho_{k(n/k)} \right) = C_k^{(n)} \left( \left\vert \psi^{(n)} \right\rangle \right).$$

Now label any $\pi \in \mathbb{Z}_n \subset S_n$ as

$$\pi^{(n)}_m : i \mapsto i + m \mod n.$$

We can then examine that, for any $m$,

$$\pi^{(n/k)}_{n/k-m} \rho_{k(n/k)} = \sum_j \sum_{a,b} \psi_{j,a} \left( \pi^{(n/k)}_m \right) \left\vert a \right\rangle \left\langle b \right\vert \psi_{j,b}^{*}$$

$$= \sum_j \sum_{a,b} \psi_{\pi^{(n/k)}_m (j,a)} \left\vert a \right\rangle \left\langle b \right\vert \psi_{j,b}^{*}$$

$$= \rho_{k(n/k)},$$

where the first equality describes the action of a permutation on the parties in $k \{n/k\}$, the second extends that permutation to the $n$ parties and rearranges using the sum over $j$, and the third uses the cyclic symmetry of $\left\vert \psi^{(n)} \right\rangle$. And so, for any $\pi \in \mathbb{Z}_n/k$,

$$\pi \rho_{k(n/k)} = \rho_{k(n/k)} \pi = \rho_{k(n/k)}.$$

Since $\rho_{k(n/k)}$ commutes with $\pi^{(n/k)}_m$, they can be simultaneously diagonalized into a basis \{ $\left\vert \phi_j \right\rangle$ \}. Since $\pi^{(n/k)}_m$ is unitary, its eigenvalues associated to each $\left\vert \phi_j \right\rangle$, can be labeled as $\lambda_j = e^{i\phi_j}$. We can then examine

$$\pi^{(n/k)}_1 \rho_{k(n/k)} = \sum_j p_j \pi^{(n/k)}_1 \left\vert \phi_j \right\rangle \left\langle \phi_j \right\vert$$

$$= \sum_j p_j e^{i\phi_j} \left\vert \phi_j \right\rangle \left\langle \phi_j \right\vert,$$

which, according to equation (9), must be equal to the original $\rho_{k(n/k)}$. This is only possible if $e^{i\phi_j} = 1$ for each $j$, implying that $\left\vert \phi_j \right\rangle$ are each CS-states.

Lastly, order the eigenstates to be decreasing in $C_k^{(n/k)} \left( \left\vert \phi_j \right\rangle \right)$. By the convexity of the pairwise concurrence, it then follows that

$$C_k^{(n/k)} \left( \rho_{k(n/k)} \right) = C_k^{(n/k)} \left( \sum_j p_j \left\vert \phi_j \right\rangle \left\langle \phi_j \right\vert \right) \leq \sum_j p_j C_k^{(n/k)} \left( \left\vert \phi_j \right\rangle \left\langle \phi_j \right\vert \right) \leq C_k^{(n/k)} \left( \left\vert \phi_1 \right\rangle \right) \leq C_k^{(n/k)} \left( \left\vert \phi_1 \right\rangle \right),$$

with the inequality being saturated by the state, (2). \qed

Interestingly, convexity was the only property of the concurrence used in the proof of Theorem 1, meaning that any entanglement measure would obey an analogous statement in CS-states.

Notably, (2) also agrees with the monogamy behavior examined in the next section, as each of $C_k^{(n)} \left( \left\vert \psi_k^{(n)} \right\rangle \right) = 0$. As a result of Theorem 1, all that remains is to find $C_k^{(n)}$ for each $n$. For $n \leq 3$, the CS subspace is equivalent to the totally symmetric one, where the maxima have previously been determined. This leads to max $C_k^{(2)} = 1$ with $\left\vert \psi_1^{(2)} \right\rangle = \frac{1}{\sqrt{2}} \left( \left\vert 00 \right\rangle + \left\vert 11 \right\rangle \right)$ and max $C_k^{(3)} = \frac{2}{3}$ with $\left\vert \psi_1^{(3)} \right\rangle = \frac{1}{\sqrt{3}} \left( \left\vert 001 \right\rangle + \left\vert 010 \right\rangle + \left\vert 100 \right\rangle \right)$. Turning to the $n \geq 4$ case, some notation needs to be established. Recall the Dicke basis \( |N \rangle \) element for totally symmetric states,

$$|N \rangle = \left( \begin{array}{c} 1 \\ \vdots \\ 1 \\ \vdots \\ 1 \end{array} \right) \prod_{z \in S_n} \prod_{j \in S_n} |n\rangle,$$

where the sum runs over all party label permutations. This naturally extends to a CS basis element in the following manner. For any particular computational basis element, a CS-state must have the same coefficient for each cyclic permutation of that basis element. Let a normalized $n$ qubit CS basis element be denoted with an overbrace,

$$\{i_1i_2...i_n\} = [Z_n \ |i_1i_2...i_n\]^{-1/2} \sum_{\pi \in \mathbb{Z}_n} \pi \{i_1i_2...i_n\},$$

(17)
where $|Z_n |i_1i_2...i_n\rangle$ denotes the cardinality of the orbit of $|i_1i_2...i_n\rangle$ under the action of the $Z_n$ cyclic permutation group. For example, consider the 4 qubit basis element,
\[
\langle 0011\rangle = \frac{1}{2} \left[ |0011\rangle + |1001\rangle + |1100\rangle + |0110\rangle \right].
\] (18)

Using this basis notation, an arbitrary 4 qubit CS-state takes the form,
\[
|\psi^{(4)}\rangle = a|0000\rangle + b|0001\rangle + c|0011\rangle + d|0101\rangle + e|0111\rangle + f|1111\rangle,
\] (19)
where $|a|^2 + |b|^2 + |c|^2 + |d|^2 + |e|^2 + |f|^2 = 1$. Likewise, an arbitrary 5 qubit CS-state would be
\[
|\psi^{(5)}\rangle = a|00000\rangle + b|00001\rangle + c|00011\rangle + d|00111\rangle + e|01111\rangle + f|11111\rangle + g|01111\rangle + h|11111\rangle,
\] (20)
with the corresponding normalization. Unfortunately, even calculating $C^{(4)}_1$ and $C^{(5)}_1$ for arbitrary states is analytically challenging, let alone maximizing over that space. Instead, the calculation will be performed on the even-X-state subspaces for $n = 4$ and $n = 5$. Even-X-states (abbreviated X-states), introduced in [16], are superpositions of only computational basis elements containing an even number of ‘1’ entries. Notably, the set of CS-states examined in [10] are a subset of the CSX-states. Arbitrary 4 and 5 qubit CSX-states then take the form,
\[
|\psi^{(4)}_X\rangle = a|0000\rangle + b|0011\rangle + c|0101\rangle + d|0111\rangle + f|1111\rangle,
\] (21)
\[
|\psi^{(5)}_X\rangle = a|00000\rangle + b|00011\rangle + c|00111\rangle + d|01011\rangle + g|01111\rangle.
\] (22)
The X-state subspace is a useful one as concurrence calculations on the space are rather simple. Two qubit reduced density matrices of X-states were shown in [10] to be of the form
\[
\rho = \begin{pmatrix} \alpha & 0 & 0 & \nu \\ 0 & \beta & \mu & 0 \\ 0 & \mu^* & \gamma & 0 \\ \nu^* & 0 & 0 & \delta \end{pmatrix}.
\] (23)
The square roots of the eigenvalues of $\rho\tilde{\rho}$ (as in the concurrence definition) [9] are the following,
\[
\lambda_i = \left\{ \sqrt{\beta\gamma} + |\mu|, \sqrt{\beta\gamma} - |\mu|, \sqrt{\alpha\delta} + |\nu|, \sqrt{\alpha\delta} - |\nu| \right\}.
\] (24)
Either the first or third term is the largest eigenvalue so the X-state concurrence is then
\[
C(|\psi_X\rangle) = 2\max \left\{ 0, |\nu| - \sqrt{\beta\gamma}, |\mu| - \sqrt{\alpha\delta} \right\}.
\] (25)
Let $C_{k,\mu}^{(n)}$ and $C_{k,\nu}^{(n)}$ indicate the possible non-zero expressions for CSX concurrence involving $\mu$ and $\nu$ respectively. Following this notation, the concurrences of arbitrary 4 and 5-qubit CSX-states can be calculated to be,

\[
\begin{align*}
C^{(4)}_{1,\mu} &= \frac{|cd^* + dc^*|}{\sqrt{2}} - 2\sqrt{\left( |a|^2 + \frac{|c|^2}{4} \right) \left( |c|^2 + |f|^2 \right)} \tag{26} \\
C^{(4)}_{1,\nu} &= |ac^* + cf^*| - \frac{1}{2} |e|^2 - |d|^2 \tag{27} \\
C^{(4)}_{2,\mu} &= |c|^2 - 2\sqrt{\left( |a|^2 + \frac{|d|^2}{2} \right) \left( |d|^2 + |f|^2 \right)} \tag{28} \\
C^{(4)}_{2,\nu} &= \sqrt{2}|ad^* + df^*| - |c|^2 \tag{29} \\
C^{(5)}_{1,\mu} &= \frac{2}{5} \left( |cd^* + da^*| + |d|^2 + |g|^2 - \sqrt{5}|a|^2 + 2|c|^2 + |d|^2 \right) \left( |c|^2 + 3|g|^2 \right) \tag{30} \\
C^{(5)}_{1,\nu} &= -\frac{2}{5} \left( \sqrt{5}ac^* + 2cg^* + dg^* \right) - |c|^2 - 2|d|^2 - |g|^2 \tag{31} \\
C^{(5)}_{2,\mu} &= \frac{2}{5} \left( |ac^* + cd^*| + |c|^2 + |g|^2 - \sqrt{5}|a|^2 + |c|^2 + 2|d|^2 \right) \left( |d|^2 + 3|g|^2 \right) \tag{32} \\
C^{(5)}_{2,\nu} &= \frac{2}{5} \left( \sqrt{5}ad^* + 2dg^* + cg^* \right) - 2|c|^2 - |d|^2 - |g|^2 \tag{33} \end{align*}
\]

In determining the maximum of $C^{(4)}_1$ and $C^{(5)}_1$ over the X-state subspace, the maximization will need to be per-
formed over both the $\mu$ and $\nu$ terms, with the overall maximum being the larger of the two resulting maxima. These maximizations are easily performed after setting all the coefficient phases equal to 0. This phase treatment maximizes each absolute value in equations (13)-(20) and simplifies the maximizations enough to readily calculate. The results are compiled in the table below. The overall maximum of $C_4^{(4)} = \frac{1}{2}$ occurs when $d = 0$ and $a = c = f = \frac{1}{\sqrt{3}}$, while the $C_5^{(5)} \approx 0.468$ maximum occurs at $a = g = 0$ and $c \approx 0.298$ $d \approx 0.955$. These maxima, while calculated only over the CSX subspace, agree with the apparent maxima in numerical results for general CS-states as shown in Figure 3 in the next section. This $C_4^{(5)}$ maximum is also a notable improvement over the lower bound established in [10].

For $n > 5$, the CSX-state concurrences can be calculated, but the spaces prove too large and complicated to maximize over analytically.

### CONSTRAINTS ON SHARED ENTANGLEMENT

The space of allowable pairwise concurrences, $\{C_{i,j}\}$ with $i$ from 1 to $n - 1$ and $j > i$, for a general $n$ qubit state is known to be constrained by monogamy relations [15]. The pairs of $\{C_k^{(n)}\}$ for CS-states obey constraints of a similar nature. Shown in Figure 1 are the $k = 1$ and $k = 2$ concurrences for $10^5$ randomly generated 4 and 5 qubit CS-states. Note that the 5 qubit concurrence space is symmetric due to the permutation properties discussed in the introduction.

| Concurrence | Maximum    |
|-------------|------------|
| $C_{1,\mu}^{(4)}$ | $\frac{1}{4}$ |
| $C_{1,\nu}^{(4)}$ | $\frac{1}{2}$ |
| $C_{1,\mu}^{(5)}$ | $\approx 0.468$ |
| $C_{1,\nu}^{(5)}$ | $\approx 0.366$ |

TABLE I: Maximum concurrences of 4 and 5 qubit CSX-states. The analytic results for $n = 5$ are the roots of complicated polynomials, so their rounded numerical values are reported instead.

This first examination demonstrates the peculiar monogamous relationship between pairwise concurrences in CS-states. It appears that for both $n = 4$ and $n = 5$, above some threshold concurrence, the other concurrence must be equal to 0. This is differs from typical monogamy relations [15][17], which also suggest that the maximally
entangled states minimize entanglement with other parties, but that states with slightly less entanglement than the maximum may share other entanglements.

The following theorem provides some analytical context to the CS-state monogamy.

**Theorem 2.** The neighborhood of states around any \(\left|\psi_2^{(4)}\right\rangle\) have \(C_1^{(4)} = 0\).

**Proof.** Consider the state,

\[
\left|\psi_2^{(4)}\right\rangle = \left|\psi_1^{(2)}\right\rangle_{1,3} \otimes \left|\psi_1^{(2)}\right\rangle_{2,4},
\]

The pure 2 qubit states with concurrence equal to 1 are equivalent to each other under local unitaries, so the set of \(\left|\psi_2^{(4)}\right\rangle\) are likewise equivalent. This implies that the entanglement properties of any \(\left|\psi_2^{(4)}\right\rangle\) can be determined by examining those of (34). Now consider altering (34) by some infinitesimal perturbation of the form of (19),

\[
\left|\psi'\right\rangle = \left|\psi_2^{(4)}\right\rangle + \epsilon \left|\psi_2^{(4)}\right\rangle,
\]

where \(\epsilon \ll 1\). To show \(C_1^{(4)} = 0\) for the above state regardless of the perturbation, we first calculate the reduced density matrix between adjacent parties,

\[
\rho_r = \frac{\epsilon}{4} + \frac{\epsilon}{2} \mathbb{R} \left[ \begin{pmatrix} 2a + 2f & b - e & b - e & 2c \\ b - e & b - e & 2\sqrt{2}d & 2c \\ 2\sqrt{2}d & 2c & e - b & e - b \\ 2c & e - b & e - b & 2a + 2f \end{pmatrix} \right] + \mathcal{O}(\epsilon^2).\]

It’s clear that only the real part of the perturbation will affect the concurrence, so continue assuming the coefficients of the perturbation are real. For simplicity, absorb \(\epsilon\) into the perturbation coefficients. Continuing in the concurrence calculation,

\[
\rho_r \tilde{\rho}_r = \frac{\epsilon}{16} \left[ \begin{pmatrix} 2b - e & b - e & b - e & 2c \\ b - e & b - e & 2\sqrt{2}d & 2c \\ 2\sqrt{2}d & 2c & e - b & e - b \\ 2c & e - b & e - b & 2a + 2f \end{pmatrix} + \mathcal{O}(\epsilon^2) \right].
\]

The square roots of the eigenvalues of this matrix are all \(\lambda_i = \frac{1}{4} \sqrt{1 + \mathcal{O}(\epsilon) + \mathcal{O}(\epsilon^2)}\). Therefore, the sum \(\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\) will certainly be negative, so the concurrence is 0.

The monogamy of CS-states is more clearly observed by examining the subconcurrence, defined as

\[
sC = \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4,
\]

where \(\lambda_i\) are the square roots of the eigenvalues of \(\rho \tilde{\rho}\) in descending magnitude, as in the concurrence definition. More simply, the subconcurrence has the same definition as the concurrence, except it doesn’t map negative sums of \(\lambda_i\) to 0. The subconcurrences of randomly generated 4 and 5 qubit CS-states are displayed in Figure 2.

![FIG. 2: Pairwise subconcurrences of 10^5 randomly generated 4 and 5 qubit CS states.](image-url)
Figure 2 clearly demonstrates the apparent thresholds in 4 and 5 qubits. For both $n = 4$ and $n = 5$, it appears that above some $k = 2$ subconcurrence, the $k = 1$ subconcurrence must be negative. Due to the symmetry discussed in the introduction, in 5-qubits, states with $k = 1$ subconcurrences above the same threshold will have negative $k = 2$ subconcurrence. For $n = 4$, however, the totally symmetric state, $|W⟩ = |0001⟩$ has the same $s_{C_1}^{(4)}$ as (34) while also having $s_{C_2}^{(4)} = \frac{1}{2}$.

Looking only at CSX-states, we found the achievable concurrence boundaries in both 4 and 5 qubits. The full analysis is presented in the appendix, but the boundaries allow for a quick determination of the concurrence thresholds in the X state subspace. The thresholds are compiled in Table II on the next page. Note that the $s_{C_1}^{(4)}$ threshold only fully holds for CSX-states. Also recall that the concurrence symmetry in 5 qubits implies that $s_{C_1}^{(5)}$ and $s_{C_2}^{(5)}$ have the same threshold.

DISCUSSION

In the search for maximally entangled state in $n$ qubit CS-states we have provided a state construction which reduces the problem to finding the states which maximize the concurrence between adjacent parties. Adjacent maxima are well understood in 2 and 3 qubits, and we have calculated the maximum for 4 and 5 qubits in the X-state subspace. Brute force calculations are obviously difficult in larger $n$, even in the X-state subspace. The development of a generalized basis for large $n$ qubit CS-states, similar to the Dicke basis for totally symmetric states, would possibly enable more general statements without quite as much raw calculation. In addition, a canonical form resulting from local unitaries which leaves the state in some simpler, yet still cyclically symmetric, state would aid in calculation. Presently, no such canonical form is known for CS-states.

The work of this paper would be interesting and simple enough to repeat with alternate pairwise entanglement measures, such as the Negativity. In particular, Theorem 1 would still hold for the Negativity and would make conclusions about adjacent entanglement equally generalizable. It would also be simple enough to extend Theorem 1 and the other entanglement permutation re-
TABLE II: Threshold concurrences of 4 and 5 qubit CSX-states. The analytic result for \( n = 5 \) is the root of a complicated polynomial, so the rounded numerical value is reported instead.

| Concurrence | Threshold |
|-------------|-----------|
| \( sC_1^{(4)} \) | \( \frac{\sqrt{7}-1}{4} \) |
| \( sC_2^{(4)} \) | \( \frac{4}{7} \) |
| \( sC_3^{(5)} \) | \( \approx 0.418 \) |

The analytic result for \( n = 5 \) is the root of a complicated polynomial, so the rounded numerical value is reported instead.

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**Appendix: X State Achievable Subconcurrence Boundaries**

To find the boundary of CSX-state subconcurrences, the boundaries of each of the pairs \( \left( sC_{1,\mu(\nu)}^{(n)}, sC_{2,\nu(\mu)}^{(n)} \right) \) need be found, with the overall boundary being a combination of the outermost boundaries from each pairing due to \( sC_k^{(n)} = \max \left\{ sC_{k,\mu}^{(n)}, sC_{k,\nu}^{(n)} \right\} \).

To simplify the search for the boundaries, note that for any 4 or 5 qubit CSX-state, the subconcurrence terms \( (26-33) \) are strictly increased by setting the coefficient phases to 0. This implies that the boundaries can be searched for among 4 and 5 qubit CSX states with purely real coefficients.

### 4 Qubits

Consider an arbitrary 4 qubit CSX state, \( (21) \), with real coefficients. The corresponding normalized state

\[
|\tilde{\psi}\rangle = \frac{1}{\sqrt{a^2 + c^2 + f^2}} \left( a |0000\rangle + c |1100\rangle + f |1111\rangle \right),
\]

has both larger or equal \( sC_1^{(4)} \) and larger or equal \( sC_2^{(4)} \).

To show this, consider either subconcurrence, \( sC \), for which it is then true that

\[
sC \left( |\tilde{\psi}\rangle \right) = sC \left( |\psi\rangle \right) \bigg|_{d=0} \geq sC \left( |\psi\rangle \right).
\]

All of which implies that the boundary of the \( \left( sC_{1,\nu}^{(4)}, sC_{2,\mu}^{(4)} \right) \) pairs can be looked for among states with \( d = 0 \). Likewise the state

\[
|\tilde{\psi}\rangle = \frac{1}{\sqrt{a^2 + f^2}} \left( a |0000\rangle + c |1100\rangle + d |1010\rangle \right)
\]

has larger or equal \( sC_1^{(4)} \), \( sC_1^{(4)} \), and \( sC_2^{(4)} \), meaning the boundaries of the \( \left( sC_{1,\mu}^{(4)}, sC_{2,\nu}^{(4)} \right) \) and \( \left( sC_{1,\nu}^{(4)}, sC_{2,\mu}^{(4)} \right) \) pairs can be found among states where \( a = f = 0 \).

Using these simplified states, the remaining coefficients can be expressed using the following spherical parametrizations,

\[
\{ a, c, f \} \rightarrow \{ \sin \theta \cos \phi, \cos \theta, \sin \theta \sin \phi \} \quad (43)
\]
\[
\{ a, c, d \} \rightarrow \{ \cos \alpha, \sin \alpha \cos \beta, \sin \alpha \sin \beta \} \quad (44)
\]
\[
\{ c, d \} \rightarrow \{ \cos \zeta, \sin \zeta \}, \quad (45)
\]

associated with the \( \left( sC_{1,\nu}^{(4)}, sC_{2,\mu}^{(4)} \right) \), \( \left( sC_{1,\mu(\nu)}^{(4)}, sC_{2,\nu(\mu)}^{(4)} \right) \), and \( \left( sC_{1,\mu}^{(4)}, sC_{2,\nu}^{(4)} \right) \) pairs respectively, where \( \{ \theta, \phi, \alpha, \beta, \zeta \} \in [0, \pi/2] \). In these parametrizations, we can define the maps,

\[
C_{\nu,\mu} : \{ \theta, \phi \} \rightarrow \left\{ sC_{1,\nu}^{(4)}, sC_{2,\mu}^{(4)} \right\} \quad (46)
\]
\[
C_{\mu(\nu),\nu} : \{ \alpha, \beta \} \rightarrow \left\{ sC_{1,\mu(\nu)}^{(4)}, sC_{2,\nu(\mu)}^{(4)} \right\} \quad (47)
\]
\[
C_{\mu,\nu} : \zeta \rightarrow \left\{ sC_{1,\mu}^{(4)}, sC_{2,\nu}^{(4)} \right\} \quad (48)
\]

according to the expressions \( (26-29) \). The boundaries of the images of these maps correspond to the boundaries of the domains, as well as the zeroes of the determinant of the Jacobians for each map. The result of these boundary determinations leaves the following two outermost boundaries,
which came from the \((sC^{(4)}_{1,\mu}, sC^{(4)}_{2,\mu})\) pairs. These boundaries are displayed in Figure 4.

\[
sC^{(4)}_{2, X} \leq \begin{cases} \frac{2}{5} \left(8 \sqrt{1 - 2 sC^{(4)}_{1, X} - 4 \left(sC^{(4)}_{1, X}\right)^2 - sC^{(4)}_{1, X} + 1} \right), & -\frac{1}{2} \leq sC^{(4)}_{1, X} \leq \frac{63}{226} \\ \frac{1}{9} \left(8 \sqrt{1 - sC^{(4)}_{1, X} - 2 \left(sC^{(4)}_{1, X}\right)^2 - 4sC^{(4)}_{1, X} - 1} \right), & \frac{63}{226} \leq sC^{(4)}_{1, X} \leq \frac{1}{2}, \end{cases}
\]

(49)

\[\bar{\psi} = \frac{1}{\sqrt{c^2 + d^2 + g^2}} \left( c \left|00011\right\rangle + d \left|00101\right\rangle + g \left|01111\right\rangle \right), \]

(50)

has larger or equal \(sC^{(5)}_{1,\mu}\) and \(sC^{(5)}_{2,\mu}\), so therefore the boundary of the \((sC^{(5)}_{1,\mu}, sC^{(5)}_{2,\mu})\) pairs can be searched for among states with \(a = 0\). For the other pairs, we will bound their subconcurrences by a sequence of lines which lie within the \((sC^{(5)}_{1,\mu}, sC^{(5)}_{2,\mu})\) boundary.

We can now parametrize the remaining coefficients of (50) as

\[
\{c, d, g\} \rightarrow \{\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta\},
\]

(51)

and define the map

\[
C_{\mu, \mu} : \{\theta, \phi\} \rightarrow \left\{sC^{(5)}_{1,\mu}, sC^{(5)}_{2,\mu}\right\},
\]

(52)

according to (30) and (32). By analyzing the boundaries of the domain and the zeroes of the determinant of the Jacobian of this map, three boundaries make up a maximal set, as plotted in Figure 5. These three boundaries are parametrized by \(\theta = \frac{\pi}{2}, \phi = 0\), and \(\phi = \frac{\pi}{2}\). The exact polynomials in \(sC^{(5)}_{1,\mu}\) and \(sC^{(5)}_{2,\mu}\) which describe these boundaries are easily determined by a Gröbner basis calculation performed on (52), but the results are quite lengthy.

\[\begin{align*}
&\text{FIG. 4: The 4 qubit CSX state subconcurrence boundaries.} \\
&\text{FIG. 5: The 5 qubit CSX state subconcurrence boundaries.}
\end{align*}\]

Turning now to the remaining subconcurrence pairings. It was shown in Table 1 that \(C^{(5)}_{1(2),\nu} \leq 0.366\). Another simple maximization shows that \(sC^{(5)}_{1,\nu} + sC^{(5)}_{2,\nu} \leq \frac{2}{5}\). These three conditions bound the \((sC^{(5)}_{1,\nu}, sC^{(5)}_{2,\nu})\) pairs to a region well within the previous boundary, as shown in Figure 6.

Lastly, the remaining two pairs, \((sC^{(5)}_{1,\mu(\nu)}, sC^{(5)}_{2,\nu(\mu)})\) can be handled together due to the symmetry in 5 qubits. Similarly to the previous pair boundary, we will find a set of lines which bound the \((sC^{(5)}_{1,\mu(\nu)}, sC^{(5)}_{2,\nu(\mu)})\) pairs. We
FIG. 6: The bounding conditions on the \( (sC_{1,\mu}^{(5)}, sC_{2,\nu}^{(5)}) \) pairs (darker blue) with the overall boundary.

can again take advantage of \( sC_{2,\nu}^{(5)} \leq 0.366 \), as well as the following two new maximizations,

\[
\begin{align*}
{sC}_{2,\nu}^{(5)} + {sC}_{1,\mu}^{(5)} &\leq \frac{47}{100} \\
{sC}_{2,\nu}^{(5)} + 2{sC}_{1,\mu}^{(5)} &\leq \frac{4}{5}
\end{align*}
\]

These three conditions bound the \( (sC_{1,\mu}^{(5)}, sC_{2,\nu}^{(5)}) \) pairs within the original boundary for \( 0 \leq sC_{1,\mu}^{(5)} \) and \( 0 \leq sC_{2,\nu}^{(5)} \), as shown in Figure 7.

Note that these conditions on the \( (sC_{1,\mu}^{(5)}, sC_{2,\nu}^{(5)}) \) do not actually fall within the original boundary for regions in \( 0.4 \leq sC_{1,\mu}^{(5)} \) and \( sC_{2,\nu}^{(5)} \leq 0 \). But given that \( sC_{2,\nu}^{(5)} \leq 0 \) for that region, the actual concurrences would be mapped to \( C_{2}^{(5)} = 0 \), where the boundaries would then agree.

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