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Werner states from diagrams

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Abstract

We present two results on multiqubit Werner states, defined to be those states that are invariant under the collective action of any given single-qubit unitary that acts simultaneously on all the qubits. Motivated by the desire to characterize entanglement properties of Werner states, we construct a basis for the real linear vector space of Werner invariant Hermitian operators on the Hilbert space of pure states; it follows that any mixed Werner state can be written as a mixture of these basis operators with unique coefficients. Continuing a study of 'polygon diagram' Werner states constructed in earlier work, with a goal to connect diagrams to entanglement properties, we consider a family of multiqubit states that generalize the singlet, and show that their 2-qubit reduced density matrices are separable.

Keywords: Werner, states, diagraming, quantum information, Werner states, entanglement

1. Introduction

Motivated by practical applications in computation, cryptography, and metrology, quantum information theory has been instrumental in shedding light on fundamental theoretical questions in physics and computer science. This includes violation of Bell inequalities and local hidden variable theories [1–3], new proofs of classical information theorems [4], and new physical principles such as information causality [5].

Certain classes of states have played significant roles in theoretical and applied developments in quantum information. This paper focuses on multiqubit Werner states, defined by their invariance under the action of local unitaries of the form $U^{\otimes n}$, for all 1-qubit unitaries U, and n is the number of qubits. Originally introduced in 1989 for two particles to distinguish between classical correlation and Bell inequality satisfaction [2], Werner states have been used

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in the description of noisy quantum channels [6], as examples in nonadditivity claims [7], for hiding classical data in quantum states [8], in the study of deterministic purification [9], and for coding in a way that protects against the loss of a qubit [10].

Significant results on the properties of Werner states include detailed understanding of structure and entanglement properties for bipartite and tripartite systems of arbitrary local dimension [2, 11] and general results on entanglement witnesses [12, 13]. In this paper, we extend our own previous work on pure and mixed Werner states of arbitrarily many qubits. In [14], we construct linear bases for the Hilbert spaces of pure Werner states, parameterized by combinatorial objects called chord diagrams. In [15], we construct mixed Werner states from another type of diagram called polygon diagrams that are directly related to properties of separability and cyclic permutational symmetry.

This paper builds on our diagram-based analyses towards further structural understanding of mixed Werner states. In section 4, we use our chord diagram basis for $2n$-qubit pure Werner states to construct a basis for the real vector space of Werner invariant Hermitian operators on the Hilbert space for n qubits; it follows that any n-qubit mixed Werner state can be written as a mixture of these basis operators with unique coefficients. Motivation for this construction comes from the success of Werner and Eggeling's precise mapping of separability regions in the space of coefficients with respect to a specific basis for tripartite Werner states [11]. Towards the goal of further connecting polygon diagrams to entanglement properties of states constructed from them, we consider a family of polygon diagram states that generalize the singlet to many qubits, and show that their 2-qubit reduced density matrices are separable in section 5. This result can be viewed as a case study related to recent work of Bernards and Gühne [16] where they show, in their study of absolutely maximally entangled states, that 2-party reduced density matrices of pure Werner states are never maximally mixed. In a distributed quantum computation scenario, these polygon Werner states provide a multipartite entanglement resource that does not allow 2-party shared entanglement, thus affording some protection against dishonest pairs of parties.

We begin with preliminary facts and notation in section 2. We give a self-contained account of our construction of pure Werner states from chord diagrams, and another construction of a family of mixed Werner states that generalize the singlet state, in section 3. Some proofs involving longer or more technical derivations are given in the appendix.

2. Preliminaries

An m-qubit pure state $|\psi\rangle$ is Werner invariant if $U^{\otimes m}|\psi\rangle \propto |\psi\rangle$ for all 1-qubit unitary operators U. An m-qubit mixed state ρ is Werner invariant if $U^{\otimes m}\rho(U^\dagger)^{\otimes m} = \rho$ for all 1-qubit unitary operators U. More generally, an operator A on m-qubit states is Werner invariant if $U^{\otimes m}A(U^\dagger)^{\otimes m} = A$ for all 1-qubit unitary operators U.

We will write $\mathcal{H}_m, \mathcal{L}(\mathcal{H}_m), \mathrm{Herm}(\mathcal{H}_m)$ to denote the Hilbert space of pure states, the space of operators on Hilbert space, and the space of Hermitian operators on Hilbert space, respectively. We will write ${\mathcal{H}_m}^{\mathcal{W}}, \mathcal{L}(\mathcal{H}_m)^{\mathcal{W}}, \mathrm{Herm}(\mathcal{H}_m)^{\mathcal{W}}$ to denote the corresponding Werner invariant subspaces. In these notations, the set of mixed states of m qubits is a subset of $\mathrm{Herm}(\mathcal{H}_m)$, and the m-qubit Werner invariant mixed states are a subset of $\mathrm{Herm}(\mathcal{H}_m)^{\mathcal{W}}$.

We write Z, X denote the 1-qubit Pauli operators $Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$, $X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ with respect to a given computational basis, and we use the notation $A^{(k)}$, where A is either Z or X, to denote the 1-qubit operator A acting on the kth qubit of a multiqubit state, i.e. $A^{(k)}$ is the operator $I^{\otimes(k-1)} \otimes A \otimes I^{(m-k)}$ in $\mathcal{L}(\mathcal{H}_m)$.

We will use the following formulas for establishing Werner invariance in sections below. An m-qubit pure state $|\psi\rangle$ is Werner invariant if the following two equations hold

$$\left(\sum_k Z^{(k)}\right)\cdot|\psi\rangle = 0 \tag{1}$$

$$\left(\sum_k X^{(k)}\right)\cdot|\psi\rangle = 0 \tag{2}$$

and an m-qubit mixed state ρ is Werner invariant if the following two equations hold.

$$\left[\left(\sum_k Z^{(k)}\right),\rho\right] = 0 \tag{3}$$

$$\left[\left(\sum_k X^{(k)}\right),\rho\right] = 0. \tag{4}$$

While these criteria for Werner invariance are well-known, we provide a proof in the appendix for the sake of self-containedness.

We will use the following notation for bit strings. Given an m-bit string $I = i_1 i_2 \ldots i_m$, we write wt$I$ to denote the Hamming weight wt$I = \sum_k i_k$. We write i_k^c to denote the complement $i_k + 1 \pmod 2$ of the kth bit i_k, and we write I_ℓ to denote the string $i_1 i_2 \ldots i_{\ell-1} i_\ell^c i_{\ell+1} \ldots i_m$, that is, the string I with only the ℓth bit complemented, and the other bits left unchanged. We write I^c to denote the string $i_1^c i_2^c \ldots i_m^c$.

Given a bit string $J = j_1, j_2, \ldots, j_d$, we write J^k to denote the kd-bit string obtained by concatenating J with itself k times. For example,

$$(011)^3 = 011011011.$$

A bit string I is called *periodic* if $I = J^k$ for some $k > 1$, and is called *aperiodic* otherwise.

3. Pure and mixed Werner state constructions from diagrams

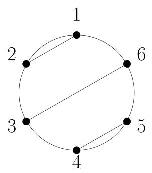
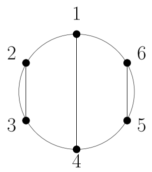
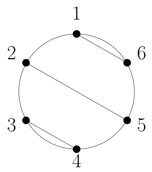
This background section provides details from previous work that is needed for the new results in the sections that follow.

It is straightforward to check that the singlet state $|s\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$ is Werner invariant. It follows that any product of singlet states is also Werner invariant. Not obvious, but true nonetheless, is that any pure Werner invariant state must be a superposition of products of singlets [14]. Thus, to describe pure Werner states, it is natural to make use of *chord diagrams* to keep track of which pairs of qubits are entangled in a product of singlets. A chord diagram with $2n$ nodes is a partition of the set $\{1, 2, \ldots, 2n\}$ into two-element subsets, called chords. The diagram is drawn with points labeled $1, 2, \ldots, 2n$ consecutively around a circle, with a line segment connecting each pair $\{a, b\}$ in the chosen partition. The figures in the left column of table 1 show examples.

For our basis construction in the next section, it will be convenient to consider *oriented* chord diagrams, where ordered pairs are used to denote chords, instead of two-element sets. We will write (a, b) do denote the directed chord starting at vertex a and ending at vertex b, and we write $|s\rangle_{a,b}$ to denote the singlet

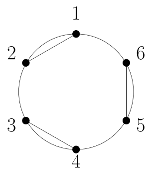
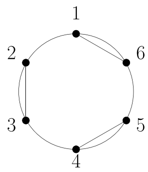
$$|s\rangle_{a,b} = \frac{1}{\sqrt{2}}\left(|0\rangle_a|1\rangle_b - |1\rangle_a|0\rangle_b\right)$$

Table 1. Bases for Werner invariant spaces for $n = 3$. The far left column shows the five 6-vertex noncrossing chord diagrams. The diagrams in the first three rows have half-turn rotational symmetry, and the diagrams in the last two rows do not (they are half-turn rotations of one another). The column with the heading '$|\mathcal{D}\rangle$' is the NCC basis for the complex 5-dimensional space of Werner invariant vectors in the Hilbert space for 6 qubits, omitting the normalizing factor $1/\sqrt{8}$. For space efficiency and readability, matrices in the column with the heading '$A_{\mathcal{D}}$' are typeset without brackets or parentheses, and the symbols '$+$', '$-$' are used to denote the entries $1/\sqrt{8}$, $-1/\sqrt{8}$, respectively. The column on the far right is a basis for the real 5-dimensional space of Werner invariant Hermitian operators on the Hilbert space for 3 qubits. The set R consists of the single diagram $\mathcal{D} = \{(1,2),(3,4),(5,6)\}$.

$\mathcal{D}$	$\lvert\mathcal{D}\rangle$	$A_{\mathcal{D}}$	Contribution to basis B
 $\{(1,2),(3,6),(4,5)\}$	$+\lvert 010011\rangle - \lvert 101100\rangle$ $-\lvert 010101\rangle + \lvert 101010\rangle$ $-\lvert 011010\rangle + \lvert 100101\rangle$ $+\lvert 011100\rangle - \lvert 100011\rangle$	$\begin{matrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & - & 0 & + & 0 & 0 & 0 \\ 0 & 0 & 0 & - & 0 & + & 0 & 0 \\ 0 & 0 & + & 0 & - & 0 & 0 & 0 \\ 0 & 0 & 0 & + & 0 & - & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{matrix}$	$A_{\mathcal{D}}$
 $\{(1,4),(2,3),(5,6)\}$	$+\lvert 001101\rangle - \lvert 110010\rangle$ $-\lvert 001110\rangle + \lvert 110001\rangle$ $-\lvert 010101\rangle + \lvert 101010\rangle$ $+\lvert 010110\rangle - \lvert 101001\rangle$	$\begin{matrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & - & + & 0 & 0 & 0 & 0 & 0 \\ 0 & + & - & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & - & + & 0 \\ 0 & 0 & 0 & 0 & 0 & + & - & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{matrix}$	$A_{\mathcal{D}}$
 $\{(1,6),(2,5),(3,4)\}$	$+\lvert 001111\rangle - \lvert 111000\rangle$ $-\lvert 001011\rangle + \lvert 110100\rangle$ $-\lvert 010101\rangle + \lvert 101010\rangle$ $+\lvert 011001\rangle - \lvert 100110\rangle$	$\begin{matrix} - & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & - & 0 & 0 & 0 \\ 0 & 0 & - & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & - & 0 \\ 0 & - & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & - & 0 & 0 \\ 0 & 0 & 0 & - & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & - \end{matrix}$	$A_{\mathcal{D}}$

(Continued.)

Table 1. (Continued.)

 $\{(1,2),(3,4),(5,6)\}$	$+\|010101\rangle - \|101010\rangle$ $-\|010110\rangle + \|101001\rangle$ $-\|011001\rangle + \|100110\rangle$ $+\|011010\rangle - \|100101\rangle$	$\begin{matrix} 0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0\\ 0&-&+&0&0&0&0&0\\ 0&0&0&0&0&-&+&0\\ 0&+&-&0&0&0&0&0\\ 0&0&0&0&0&+&-&0\\ 0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0 \end{matrix}$	$\frac{A_{\mathcal{D}}+A^T_{\mathcal{D}}}{2}$, $\frac{A_{\mathcal{D}}-A^T_{\mathcal{D}}}{2i}$
 $\{(1,6),(2,3),(4,5)\}$	$+\|001011\rangle - \|110100\rangle$ $-\|001101\rangle + \|110010\rangle$ $-\|010011\rangle + \|101100\rangle$ $+\|010101\rangle - \|101010\rangle$	$\begin{matrix} 0&0&0&0&0&0&0&0\\ 0&0&-&0&+&0&0&0\\ 0&0&+&0&-&0&0&0\\ 0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0\\ 0&0&0&-&0&+&0&0\\ 0&0&0&+&0&-&0&0\\ 0&0&0&0&0&0&0&0 \end{matrix}$	(None)

associated to the directed chord (a,b). Given an oriented chord diagram $\mathcal{D} = \{(a_k,b_k)\}_{1\leqslant k\leqslant n}$, we define the state $|\mathcal{D}\rangle$ to be the product of singlets

$$|\mathcal{D}\rangle = \bigotimes_{1\leqslant k\leqslant n} |s\rangle_{a_k,b_k}.$$

In the Hilbert space $(\mathbb{C}^2)^{\otimes 2n}$ of the composite system of $2n$ qubits in order $\{1,2,\ldots,2n\}$, the orientation reversal of a chord flips the sign of a diagram state. That is, if $\mathcal{D},\mathcal{D}'$ share all but one of the same oriented chords, but (a,b) is a chord in $\mathcal{D}$ and (b,a) is a chord in $\mathcal{D}'$, we have $|\mathcal{D}\rangle = -|\mathcal{D}\rangle'$. The coefficients c_K in the expression $|\mathcal{D}\rangle = \sum_K c_K|K\rangle$ for $|\mathcal{D}\rangle$ in the computational basis parameterized by $2n$-bit strings $K = k_1k_2\ldots k_{2n}$ are given by

$$c_K = \begin{cases} \prod_{\ell=1}^{n}(-1)^{k_{a_\ell}} & \text{if } k_{a_\ell} = k^c_{b_l} \text{ for } 1\leqslant \ell \leqslant n \\ 0 & \text{otherwise} \end{cases}. \tag{5}$$

A chord diagram is said to be *noncrossing* if there are no intersections of chords in the geometric picture. We will write NCC to denote the set of all $2n$-node noncrossing chord diagrams, where n will be understood from context, where each chord $\{a,b\}$ with $a < b$ has the orientation (a,b). It is a remarkable fact [14] the set of singlet products corresponding to NCC form a $\mathbb{C}$-linear basis for pure Werner states. Table 1 shows the five noncrossing chord diagrams for 6 qubits.

We will use the following singlet product state in our constructions for mixed Werner states in the next section. We define the 'pizza diagram' $\mathcal{P}_0$ to be the chord diagram $\mathcal{P}_0 = \{(i,i+n)\colon 1\leqslant i\leqslant n\}$. See figure 1. For convenience, we rescale the state $|\mathcal{P}_0\rangle$ to define the

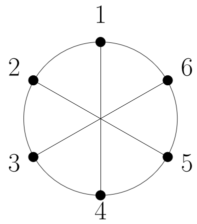


Figure 1. The 'pizza' diagram $\mathcal{P}_0$ for $2n = 6$ qubits. The unnormalized pizza state is $|P\rangle = |000111\rangle - |111000\rangle - |001110\rangle + |110001\rangle - |010101\rangle + |101010\rangle + |011100\rangle - |100011\rangle$.

(unnormalized) $2n$-qubit, Werner invariant 'pizza state' $|P\rangle = 2^{n/2}|\mathcal{P}_0\rangle$. Using notation from section 2 above, the pizza state can be expressed as follows.

$$|P\rangle = \sum_I (-1)^{\mathrm{wt}I} |I\rangle |I^c\rangle = 2^{n/2} |\mathcal{P}_0\rangle . \tag{6}$$

Next, we construct a family of mixed Werner states ρ_m that generalize the density matrix $\rho_2 = |s\rangle\langle s|$ of the singlet[1]. The first step is to construct a pure state $C(I)$ for every aperiodic m-bit string $I = i_1 i_2 \cdots i_m$, given by

$$C(I) = \frac{1}{\sqrt{m}} \sum_{k=0}^{m-1} \omega^k \left|\pi^k I\right\rangle \tag{7}$$

where $\omega = e^{2\pi i/m}$ and π is the cyclic permutation of $\{1, 2, \ldots, m\}$ given by $j \to j-1 \pmod m$. For example, we have

$$C(001) = \frac{1}{\sqrt{3}}(|001\rangle + e^{\frac{2\pi i}{3}} |010\rangle + e^{\frac{4\pi i}{3}} |100\rangle).$$

(Note that if I is periodic, then $C(I) = 0$, and is therefore not a state.) Now we define ρ_m by

$$\rho_m = \frac{1}{A(m)} \sum_{\text{aperiodic } I} C(I) C(I)^\dagger \tag{8}$$

where $A(m)$ is the number of aperiodic m-bit strings [17]. It is easy to check that $\rho_2 = |s\rangle\langle s|$ is the density matrix for the singlet state, and it is a fact [15] that ρ_m is Werner invariant for all $m \geqslant 1$.

4. A mixed Werner basis construction

In this section we construct a basis for the real vector space $\mathrm{Herm}(\mathcal{H}_n)^{\mathcal{W}}$. It follows that any n-qubit mixed Werner state can be written uniquely as an $\mathbb{R}$-linear combination of matrices in this set. The overall strategy is to map a known basis for $2n$-qubit pure Werner states (the noncrossing chord diagram states) to a basis of operators on the Werner invariant subspace of Hermitian operators n-qubit state space.

[1] The states ρ_m appear as tensor factors in a diagrammatic construction for mixed Werner states that generalizes the chord diagram construction for pure Werner states. The results of section 5 do not require the full polygon state construction, so we limit our discussion to only the necessary details for ρ_m.

To begin, let $\mathcal{H} = \mathcal{H}_{2n} = (\mathbb{C}^2)^{\otimes n} \otimes (\mathbb{C}^2)^{\otimes n}$ denote the Hilbert space of $2n$-qubit states with computational basis $\{|I\rangle|J\rangle\}$, where I, J each range over the set of all n-bit strings. Let $(\mathcal{H}_{2n})_{\mathbb{R}}$ denote the subspace of states with real coefficients in the computational basis,

$$(\mathcal{H}_{2n})_{\mathbb{R}} = \left\{ \sum_{IJ} c_{IJ} |I\rangle |J\rangle : c_{IJ} \in \mathbb{R} \right\}.$$

Let m denote the $\mathbb{R}$-linear map $m\colon (\mathcal{H}_{2n})_{\mathbb{R}} \to \mathcal{L}(\mathcal{H}_n)$ that takes the computational basis vector $|I\rangle|J\rangle$ to $|I\rangle\langle J|$ (note that m is *not* $\mathbb{C}$-linear). Observe that $|\mathcal{D}\rangle$ lies in $(\mathcal{H}_{2n})_{\mathbb{R}}$ for any chord diagram (crossing or noncrossing), so that $m(|\mathcal{D}\rangle)$ is defined.

Next, we establish useful properties of the 'pizza operator' $m(|P\rangle)$ obtained by applying m to the (unnormalized) pizza state $|P\rangle$. The symbol Y denotes the Pauli operator $Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$.

Proposition 1 (Properties of the pizza operator). *The following hold.*

(i) $m(|P\rangle) = \sum_I (-1)^{\mathrm{wt}I} |I\rangle\langle I^c|$
(ii) $m(|P\rangle)^T = (-1)^n m(|P\rangle)$
(iii) $m(|P\rangle) = (iY)^{\otimes n} = 2^{n/2} m(|s\rangle)^{\otimes n}$
(iv) $m(|P\rangle)^2 = (-1)^n \mathrm{Id}$.

Proof. For (i), apply the definition of m to the expression (6) for the pizza state. For (ii), use $\mathrm{wt}I + \mathrm{wt}I^c = n$, so $(-1)^{wtI^c} = (-1)^n(-1)^{\mathrm{wt}I}$. Checking (iii) is a straightforward computation, and (iv) follows from $(iY)^2 = -\mathrm{Id}$. □

The next proposition establishes key properties of products $m(|P\rangle)m(|\mathcal{D}\rangle)$.

Proposition 2. *Let $\mathcal{D}$ be any chord diagram, crossing or noncrossing. The following hold.*

(i) $m(|P\rangle)m(|\mathcal{D}\rangle) = m(|\mathcal{D}\rangle)m(|P\rangle)$
(ii) $m(|P\rangle)m(|\mathcal{D}\rangle)$ *is Werner invariant.*

Proof. The proof of (i) requires only simple observations about products of singlets. The proof of (ii) uses Werner invariance criteria (1)–(4) to verify that $m(|P\rangle)m(|\mathcal{D}\rangle)$ is Werner invariant. Details are given in the appendix. □

In the remainder of this section, we describe how to construct a basis for $\mathrm{Herm}(\mathcal{H}_n)^{\mathcal{W}}$ from the Werner invariant matrices in part (ii) of proposition 2 above. For compactness and readability, let

$$A_{\mathcal{D}} := m(|P\rangle)m(|\mathcal{D}\rangle).$$

We will show that there are two possibilities for $A_{\mathcal{D}}$, depending on whether $\mathcal{D}$ has half-turn rotational symmetry. For $\mathcal{D} = \{(a_k, b_k)\colon 1 \leqslant k \leqslant n\}$, we define $R_{180}\mathcal{D}$ by

$$R_{180}\mathcal{D} = \{(a_k + n, b_k + n)\colon 1 \leqslant k \leqslant n\}$$

where addition in the last expression is taken mod $2n$. To say that a diagram $\mathcal{D}$ has half-turn rotational symmetry means that $\mathcal{D}, R_{180}\mathcal{D}$ are equal as unoriented chord diagrams, which is the same as $|\mathcal{D}\rangle = \pm|R_{180}\mathcal{D}\rangle$. We will show that

- $A_{\mathcal{D}}$ is symmetric if $\mathcal{D}$ has half-turn symmetry, and
- $A_{\mathcal{D}}, A_{R_{180}\mathcal{D}}$ are distinct and are transposes of one other (up to a sign) if $\mathcal{D}$ does not have half-turn symmetry.

We then construct a set of Hermitian matrices from linear combinations of the $A_{\mathcal{D}}$, and finally, we argue why this set forms a basis. We begin with a proposition that relates half-turn rotation and matrix transpose.

Proposition 3. *Let $\mathcal{D}$ be an oriented $2n$-vertex chord diagram, crossing or noncrossing. We have the following.*

$$m(|R_{180}\mathcal{D}\rangle) = m(|\mathcal{D}\rangle)^T. \tag{9}$$

Proof. Let $\mathcal{D} = \{(a_k, b_k)\}_k$ so that $R_{180}\mathcal{D} = \{(a_k+n, b_k+n)\}_k$.

Given a $2n$-bit string $K = k_1k_2\ldots k_{2n}$, let $R_{180}K$ denote the string $R_{180}K = k_{1+n}k_{2+n}\ldots k_{2n+n}$, where addition in the subscripts is taken mod $2n$. Thus if $K = IJ$ is the concatenation of n-bit strings I, J, then $R_{180}K = JI$.

Let $|\mathcal{D}\rangle = \sum_K c_K |K\rangle$ be the expansion of $|\mathcal{D}\rangle$ in the computational basis. If a $2n$-bit string $K = k_1k_2\ldots k_{2n}$ meets the criterion

$$k_{a_\ell} = k^c_{b_\ell}, 1 \leqslant \ell \leqslant n$$

then the bit string $K' = R_{180}K$ satisfies

$$k'_{a_\ell} = k_{a_\ell - n} = k^c_{b_\ell - n} = (k'_{b_\ell})^c, 1 \leqslant \ell \leqslant n.$$

Using equation (5), we have

$$|R_{180}\mathcal{D}\rangle = \sum_K c_K |R_{180}K\rangle = \sum_{IJ} c_{IJ} |J\rangle\langle I| = m(|\mathcal{D}\rangle)^T.$$

□

The next proposition establishes a detail about the sign in the equation $|\mathcal{D}\rangle = \pm|R_{180}\mathcal{D}\rangle$ for diagrams $\mathcal{D}$ with half-turn symmetry. We begin with a lemma.

Lemma 1. *Let $\mathcal{D}$ be a $2n$-vertex chord diagram, crossing or noncrossing. The number of chords that cross the 'midline', that is, the chords that have one vertex in the set $\{1,2,\ldots,n\}$ and the other vertex in the set $\{n+1, n+2,\ldots,2n\}$, has the same parity as n.*

Proof. Let c be the number of chords that have one vertex in the first half $\{1,2,\ldots,n\}$ of the vertices and one vertex in the second half $\{n+1, n+2,\ldots,2n\}$ of the vertices. The number of chords that have both vertices in the first half must be equal to the number of chords that have both vertices in the second half, so $n-c$ is even. □

Proposition 4. *Suppose that $\mathcal{D}$ has half-turn symmetry, so that $|\mathcal{D}\rangle = \pm|R_{180}\mathcal{D}\rangle$. Then the sign is determined by n, and we have*

$$|\mathcal{D}\rangle = (-1)^n |R_{180}\mathcal{D}\rangle. \tag{10}$$

Proof. Let c be the number of chords in $\mathcal{D}$ that join vertices in the first half $\{1,2,\ldots,n\}$ with vertices in the second half $\{n+1, n+2,\ldots,2n\}$. By lemma 1, c has the same parity as n, so we have $(-1)^c = (-1)^n$. Each oriented chord (a,b) in $\mathcal{D}$ is mapped to $(a+n, b+n)$ in $R_{180}\mathcal{D}$. The number of orientation reversals accounts for the global sign $(-1)^c = (-1)^n$. □

Applying m to both sides of (10), and then multiplying both sides by $m(|P\rangle)$, we have the following corollary.

Corollary 1. *If $\mathcal{D}$ has half-turn symmetry, then we have the following.*

$$m(|\mathcal{D}\rangle) = (-1)^n m(|R_{180}\mathcal{D}\rangle) \tag{11}$$

$$A_{\mathcal{D}} = (-1)^n A_{R_{180}\mathcal{D}}. \tag{12}$$

Proposition 5. *Let $\mathcal{D}$ be an oriented $2n$-vertex chord diagram, crossing or noncrossing. We have the following.*

$$A_{R_{180}\mathcal{D}} = (-1)^n A_{\mathcal{D}}^T \tag{13}$$

Proof. Multiplying both sides of (9) on the left by $m(|P\rangle)$, we have

$$m(|P\rangle)m(|R_{180}\mathcal{D}\rangle) = m(|P\rangle)m(|\mathcal{D}\rangle)^T.$$

Using proposition 1, part (ii), the right side becomes

$$\begin{aligned}(-1)^n m(|P\rangle)^T m(|\mathcal{D}\rangle)^T &= (-1)^n \left[m(|\mathcal{D}\rangle)m(|P\rangle)\right]^T \\ &= (-1)^n \left[m(|P\rangle)m(|\mathcal{D}\rangle)\right]^T \text{(by proposition 2, part (i))}.\end{aligned}$$

We conclude that (13) holds. □

The following corollary follows immediately from corollary 1 and proposition 5.

Corollary 2. *If $\mathcal{D}$ has half-turn symmetry, then $A_{\mathcal{D}} = A_{\mathcal{D}}^T$.*

Now we construct a set of Hermitian matrices. For every $\mathcal{D}$ in NCC, let $S_{\mathcal{D}}$ denote the set

$$S_{\mathcal{D}} = \left\{\frac{A_{\mathcal{D}} + A_{\mathcal{D}}^T}{2}, \frac{A_{\mathcal{D}} - A_{\mathcal{D}}^T}{2i}\right\}.$$

Because the $A_{\mathcal{D}}$ have real entries, the matrices in $S_{\mathcal{D}}$ are Hermitian. To extract a basis from the collection $\bigcup_{\mathcal{D}\in \mathrm{NCC}} S_{\mathcal{D}}$, we need to weed out linear dependencies that arise from the fact that $A_{\mathcal{D}}^T = A_{R_{180}\mathcal{D}}$ (proposition 5). We categorize diagrams in NCC into two types, corresponding to when the underlying unoriented chord diagram either does have or does not have half-turn rotational symmetry,

$$\begin{aligned}\mathrm{NCC}_{\mathrm{symm}} &= \{\mathcal{D} \in \mathrm{NCC}\colon\ |\mathcal{D}\rangle = \pm|R_{180}\mathcal{D}\rangle\} \\ \mathrm{NCC}_{\mathrm{nonrot}} &= \{\mathcal{D} \in \mathrm{NCC}\colon\ |\mathcal{D}\rangle \neq \pm|R_{180}\mathcal{D}\rangle\}.\end{aligned}$$

The figures in the left column of table 1 show examples of each of these types.

If $\mathcal{D} \in \mathrm{NCC}_{\mathrm{symm}}$, then $A_{\mathcal{D}}$ is real symmetric by corollary 2, so $S_{\mathcal{D}} = \{A_{\mathcal{D}}, 0\}$. If $\mathcal{D} \in \mathrm{NCC}_{\mathrm{nonrot}}$, then $S_{\mathcal{D}}$ is a set of two nonzero Hermitian matrices. But we have redundancies: let $\mathcal{E}$ be the *unoriented* noncrossing chord diagram with the same diagram as $R_{180}\mathcal{D}$, and give $\mathcal{E}$ the standard orientation (so that the chord $\{a,b\}$ is oriented (a,b) with $a<b$) so that $\mathcal{E}$ is in NCC. Then the vectors in the set $S_{\mathcal{E}}$ are the same, up to sign, as the vectors in $S_{\mathcal{D}}$, so that the sets $S_{\mathcal{D}}, S_{\mathcal{E}}$ have the same linear span. To eliminate these redundancies, let R be a set consisting of a choice of one of the two $\mathrm{NCC}_{\mathrm{nonrot}}$ diagrams $\mathcal{D}, \mathcal{E}$ for each pair of the type just described. The choice can be arbitrary, but here is one way to construct R explicitly. Write $\mathcal{D}$ in NCC as a string of indices $a_1, b_1, a_2, b_2, \ldots, a_n, b_n$, where $\{a_k, b_k\}$ are the unoriented chords in $\mathcal{D}$ with $a_k < b_k$ for all k, and $a_1 < a_2 < \cdots < a_n$. Then write $\mathcal{D} < \mathcal{D}'$ to indicate that $\mathcal{D}$ comes before $\mathcal{D}'$ in lexicographical order. Now we can define the set R by

$$R = \{\mathcal{D} \in \mathrm{NCC}_{\mathrm{nonrot}}\colon\ \mathcal{D} < R_{180}\mathcal{D}\}.$$

Now we assemble carefully chosen elements from the sets $S_{\mathcal{D}}$. Let B be the set

$$B = \{A_{\mathcal{D}}\colon\ \mathcal{D} \in \mathrm{NCC}_{\mathrm{symm}}\} \cup \left\{\frac{A_{\mathcal{D}} + A_{\mathcal{D}}^T}{2}, \frac{A_{\mathcal{D}} - A_{\mathcal{D}}^T}{2i} : \mathcal{D} \in R\right\}. \tag{14}$$

To complete the argument that B satisfies the requirements for our basis construction, we count dimensions. The dimension of ${\mathcal{H}_{2n}}^{\mathcal{W}}$ is the Catalan number $C_n = \frac{1}{n+1}\binom{2n}{n}$ [14]. The set $\{|\mathcal{D}\rangle : \mathcal{D} \in \mathrm{NCC}\}$ is a $\mathbb{C}$-basis for ${\mathcal{H}_{2n}}^{\mathcal{W}}$, so the cardinality of the set NCC is C_n. The dimension of the space $\mathrm{Herm}(\mathcal{H}_n)^{\mathcal{W}}$ is also the Catalan number C_n [15]. The real linear transformation ${\mathcal{H}_{2n}}^{\mathcal{W}} \to \mathrm{Herm}(\mathcal{H}_n)^{\mathcal{W}}$ taking $|\mathcal{D}\rangle$ to $A_{\mathcal{D}}$ is nonsingular. For $\mathcal{D} \in R$, we have $A^T_{\mathcal{D}} = \pm A_{R_{180}\mathcal{D}}$, and the transformation determined by

$$(A_{\mathcal{D}}, A^T_{\mathcal{D}}) \to \left(\frac{A_{\mathcal{D}} + A^T_{\mathcal{D}}}{2}, \frac{A_{\mathcal{D}} - A^T_{\mathcal{D}}}{2i}\right)$$

is invertible. Thus, the set B is a set of independent Hermitian operators with cardinality C_n. We conclude that B is a basis for $\mathrm{Herm}(\mathcal{H}_n)^{\mathcal{W}}$. This completes the basis construction. We record the result with the following theorem. Table 1 shows details for the example $n = 3$.

Theorem 1 (A basis for *n*-qubit Werner mixed states). *The set B (given by (14) above) is a basis for the real vector space* $\mathrm{Herm}(\mathcal{H}_n)^{\mathcal{W}}$. *Any n-qubit Werner invariant density matrix is a unique* $\mathbb{R}$*-linear combination of elements in this basis.*

5. Polygon states: 2-party reduced density matrices

In this section we show that any 2-party reduced density matrix of the Werner state ρ_m (equation (8)) is separable for $m \geqslant 3$.

Because partial trace commutes with the local unitary action, Werner invariance of a mixed state is inherited by all of its reduced density matrices. In particular, any 2-qubit reduced density matrix of a Werner state is also a Werner state, which can be written in the form

$$\rho = \lambda \frac{\mathrm{Id}}{4} + (1-\lambda)\,|s\rangle\,\langle s|$$

for some $0 \leqslant \lambda \leqslant 4/3$. The state ρ is entangled if $\rho_{00,00} < 1/6$ and ρ is separable if $\rho_{00,00} \geqslant 1/6$ [2, 18].

Choose two qubits a, b, $1 \leqslant a < b \leqslant m$, and let ρ be the 2-qubit Werner state

$$\rho = \rho_m^{a,b} = \mathrm{tr}_{(\text{all but}\, a,b)}\,\rho_m.$$

It will be convenient to use the following labels (see section 2 for the definition of aperiodic m-bit string),

$$\begin{aligned} A(m) &= \text{number of aperiodic } m\text{-bit strings} \\ P(m) &= \text{number of periodic } m\text{-bit strings} \\ A_{00}(m) &= \text{number of aperiodic } m\text{-bit strings with 00 in } a,b \\ P_{00}(n) &= \text{number of periodic } m\text{-bit strings with 00 in } a,b. \end{aligned}$$

We shall make use of the following elementary relationships.

$$2^m = A(m) + P(m) \tag{15}$$

$$2^{m-2} = A_{00}(m) + P_{00}(m) \tag{16}$$

$$P_{00}(m) \leqslant P(m) \tag{17}$$

$$P(m) = \sum_{d|m, d<m} A(d) \tag{18}$$

$$P(m) \leqslant \sum_{i=1}^{\lfloor m/2 \rfloor} A(i) \leqslant \sum_{i=0}^{\lfloor m/2 \rfloor} 2^i = 2^{\lfloor m/2 \rfloor + 1} - 1. \tag{19}$$

The left-most inequality in (19) comes from the fact that the number of divisors of m is upper-bounded by $\lfloor m/2 \rfloor$.

We begin by obtaining an expression for $\rho_{00,00}$. Suppose an m-bit string I is aperiodic, with $i_a = i_b = 0$. From the definition (7) for $C(I)$, we have

$$C(I)C(I)^\dagger = \frac{1}{m} \sum_{k,\ell=0}^{m-1} \omega^{k-\ell} \left|\pi^k I\right\rangle \left\langle \pi^\ell I\right|. \tag{20}$$

The only term in the sum on the right side that gives a nonzero contribution to the partial trace over all qubits but a,b is for $k = \ell = 0$, so we have

$$\langle 0_a 0_b | \operatorname{tr}_{(\text{all but}\, a,b)} C(I)C(I)^\dagger |0_a 0_b\rangle = \frac{1}{m}. \tag{21}$$

From (20), it is easy to see that $C(I)C(I)^\dagger = C(\pi^k I)C(\pi^k I)^\dagger$ for $0 \leqslant k \leqslant m-1$, so (21) becomes

$$\langle 0_a 0_b | \operatorname{tr}_{(\text{all but}\, a,b)} \sum_{k=0}^{m-1} C(\pi^k I)C(\pi^k I)^\dagger |0_a 0_b\rangle = 1. \tag{22}$$

From definition (8), it follows that

$$\rho_{00,00} = \frac{A_{00}(m)}{A(m)}. \tag{23}$$

Applying (15)–(19), we have

$$\begin{aligned}
\rho_{00,00} &= \frac{A_{00}(m)}{A(m)} && (24)\\
&= \frac{2^{m-2} - P_{00}(m)}{2^m - P(m)} && (25)\\
&\geqslant \frac{2^{m-2} - P(m)}{2^m} && (26)\\
&\geqslant \frac{2^{m-2} - 2^{\lfloor m/2 \rfloor + 1} + 1}{2^m} && (27)\\
&\geqslant \frac{2^{m-2} - 2^{\lfloor m/2 \rfloor + 1}}{2^m} && (28)\\
&= \frac{1}{4} - 2^{\lfloor m/2 \rfloor + 1 - m} && (29)\\
&= \begin{cases} \frac{1}{4} - 2^{(2-m)/2} & m\,\text{even} \\ \frac{1}{4} - 2^{(1-m)/2} & m\,\text{odd} \end{cases}. && (30)
\end{aligned}$$

It is clear that (30) increases as m increases. It is easy to check that (30) is equal to $3/16 > 1/6$ for $m = 9, 10$, so therefore (30) is larger than $1/6$ for $m \geqslant 9$. Table 2 shows that $\rho^{a,b}_{00,00} \geqslant 1/6$ for all possibilities for a,b, for $3 \leqslant m \leqslant 8$. We record the result of this section as the following theorem.

Theorem 2. *Let ρ_m denote the m-qubit mixed Werner state (8) for some $m \geqslant 3$. Let a,b be any two qubits $1 \leqslant a,b \leqslant m$, and let $\rho = \rho^{a,b}_m$ be the 2-qubit reduced density matrix of ρ_m is the subsystem consisting of qubits a,b. Then ρ is separable.*

Table 2. Values of $\rho_{00,00}$ for $3 \leqslant m \leqslant 8$ showing separability (any value $\geqslant 1/6$ implies $\rho_{00,00}$ is separable). Table values depend only on the distance $|a-b|$ because of the cyclic symmetry of ρ_m.

m	$\|a-b\|$	$\rho_{00,00}$
3	1	$1/6 \approx 0.1667$
4	1	$1/4 \approx 0.2500$
4	2	$1/6 \approx 0.1667$
5	1	$7/30 \approx 0.2333$
5	2	$7/30 \approx 0.2333$
6	1	$7/27 \approx 0.2593$
6	2	$13/54 \approx 0.2407$
6	3	$2/9 \approx 0.2222$
7	1	$31/126 \approx 0.2540$
7	2	$31/126 \approx 0.2460$
7	3	$31/126 \approx 0.2460$
8	1	$1/4 \approx 0.2500$
8	2	$1/4 \approx 0.2500$
8	3	$1/4 \approx 0.2500$
8	4	$7/30 \approx 0.2333$

6. Outlook

The eventual goal for constructing a basis for mixed Werner states is to characterize entanglement properties and identify resource states in terms of coefficients with respect to that basis. A first step will be to determine constraints on coefficients that correspond to *states*, i.e. operators that are positive semidefinite and have trace 1. There will be two immediately interesting questions: in what ways can we use the bases constructed in section 4 for $n \geqslant 3$ qubits to generalize or extend Werner and Eggeling's basis in [11]? Second, can we generalize and extend the basis construction to qudits?

The separability result in section 5 for 2-qubit reduced density matrices of Werner states ρ_m provides motivation to seek further results in characterizing separability properties for mixtures of polygon diagram states, constructed in [15]. We hope to identify distributed entanglement protocols that will exploit these states.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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Appendix. Proofs of propositions

Proof Werner invariance criteria. Formulas (1)–(4) are special cases of more general formulas for the action of the Lie algebra of the local unitary group on pure and mixed states.

(For example, see [19]. See [20] for a connection with angular momentum.) For the sake of self-containedness, here is a proof.

The Lie algebra $L(SU(2))$ of the special unitary group $SU(2)$ is the real vector space of 2×2 skew-Hermitian matrices with trace zero, and is generated (by real linear combinations and the bracket operation) by the operators iZ, iX. Given a group action $\Phi\colon SU(2)\times V\to V$ on a vector space V, there is a Lie algebra action $L(\Phi)\colon L(SU(2))\times V\to V$ on V given by by $L(\Phi)(M)v = \frac{\mathrm{d}}{\mathrm{d}t}\big|_{t=0}\Phi(\exp(tM))v$, where $M = i(aX+bY+cZ)$ for some real coefficients a,b,c, and Y is the Pauli Y operator. If both generators iZ, iX annihilate a vector v in V, then v is fixed by $\exp(it(aX+bY+cZ)$ for all real t. To obtain the results in the lemma, we apply this basic observation to the actions of $SU(2)$ on $\mathcal{H}_m$ and $\mathcal{L}(\mathcal{H}_m)$ by the standard local unitary actions

$$\Phi_{\text{pure}}(U)\,|\psi\rangle = U^{\otimes m}\,|\psi\rangle \tag{31}$$

$$\Phi_{\text{mixed}}(U)\rho = U^{\otimes m}\rho(U^{\dagger})^{\otimes m}. \tag{32}$$

The Werner invariance conditions in the lemma arise by taking derivatives on the right sides of the following equations.

$$0 = L(\Phi_{\text{pure}})(iZ)\,|\psi\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0}\exp(itZ)^{\otimes m}\,|\psi\rangle$$

$$0 = L(\Phi_{\text{pure}})(iX)\,|\psi\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0}\exp(itX)^{\otimes m}\,|\psi\rangle$$

$$0 = L(\Phi_{\text{mixed}})(iZ)\rho = \frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0}\exp(itZ)^{\otimes m}\rho\exp(-itZ)^{\otimes m}$$

$$0 = L(\Phi_{\text{mixed}})(iX)\rho = \frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0}\exp(itX)^{\otimes m}\rho\exp(-itX)^{\otimes m}.$$

Finally, we observe that if a pure state $|\psi\rangle$ is fixed by every U in $SU(2)$ acting by (31), then $|\psi\rangle$ is fixed, up to a phase factor, by any V in $U(2)$, since any particular $V\in U(2)$ can be written $e^{i\theta}U$ for some real θ and some $U\in SU(2)$. (No such phase adjustment is necessary for (32).) This concludes the proof.

The following lemma gives computationally useful forms for the Werner invariance criteria (1)–(4). The proof is straightforward checking. For more general formulas for which these are special cases, see [19].

Lemma 2 (Detailed forms of Werner invariance criteria). *Let* $|\psi\rangle = \sum_I c_I\,|I\rangle$ *and let* $\rho = \sum_{I,J}\rho_{I,J}\,|I\rangle\,\langle J|$ *be a pure state and a mixed state, respectively, of m-qubits, with respect to the computational basis. The following hold.*

$$\left(\sum_k Z^{(k)}\right)\cdot|\psi\rangle = \sum_I\left(\sum_k(-1)^k\right)c_I\,|I\rangle \tag{33}$$

$$\left(\sum_k X^{(k)}\right)\cdot|\psi\rangle = \sum_I\left(\sum_k c_{I_k}\right)|I\rangle \tag{34}$$

$$\left[\left(\sum_k Z^{(k)}\right),\rho\right] = \sum_{IJ}\rho_{IJ}\left(\sum_{k:\ i_k\neq j_k}(-1)^{i_k}\right)|I\rangle\,\langle J| \tag{35}$$

$$\left[\left(\sum_k X^{(k)}\right), \rho\right] = \sum_{IJ}\left(\sum_{k,\ell=1}^{n}(\rho_{I_k,J} - \rho_{I,J_\ell})\right)|I\rangle\langle J|. \tag{36}$$

Proof of proposition 2. Let $|\mathcal{D}\rangle = \sum_{K,J} c_{KJ}|K\rangle|J\rangle$. Because $|\mathcal{D}\rangle$ is a product of singlets, we have

$$n = \text{wt}K + \text{wt}J \text{ and} \tag{37}$$

$$c_{K^cJ^c} = (-1)^n c_{KJ} \tag{38}$$

for all K, J such that $c_{KJ} \neq 0$. From (37) we have

$$(-1)^{\text{wt}K} = (-1)^n(-1)^{\text{wt}J} \tag{39}$$

for all K, J such that $c_{KJ} \neq 0$. As a special case of (37), we have

$$n = \text{wt}I + \text{wt}I^c \tag{40}$$

for all I in the expression $m(|P\rangle) = \sum_I (-1)^{\text{wt}I}|I\rangle\langle I^c|$ (part (i) of proposition 1). □

(Proof of statement (i)) We have

$$m(|P\rangle)m(|\mathcal{D}\rangle) = \left(\sum_I (-1)^{\text{wt}I}|I\rangle\langle I^c|\right)\left(\sum_{K,J} c_{KJ}|K\rangle\langle J|\right) \tag{41}$$

$$= \sum_{I,J}(-1)^{\text{wt}I} c_{I^cJ}|I\rangle\langle J| \tag{42}$$

$$= \sum_{K,J}(-1)^{\text{wt}K} c_{K^cJ}|K\rangle\langle J| (\text{substitute} I \leftrightarrow K)$$

$$= \sum_{K,J}(-1)^n(-1)^{\text{wt}K}(-1)^n c_{K^cJ^c}|K\rangle\langle J^c| (\text{substitute} J \leftrightarrow J^c)$$

$$= \sum_{K,J}(-1)^{\text{wt}J} c_{KJ}|K\rangle\langle J^c| (\text{using (38) and (using (39)}$$

$$= \left(\sum_{K,J} c_{KJ}|K\rangle\langle J|\right)\left(\sum_I (-1)^{\text{wt}I}|I\rangle\langle I^c|\right)$$

$$= m(|\mathcal{D}\rangle)m(|P\rangle).$$

(Proof of statement (ii)) To show Werner invariance of $m(|P\rangle)m(|\mathcal{D}\rangle)$, we check that conditions (35), (36) hold for the expression (42). Because (37) and (40) are satisfied in (41), we must have

$$n = \text{wt}I + \text{wt}J$$

in (42) for every $|I\rangle\langle J|$ term with nonzero coefficient. From this it follows that

$$\sum_{k:\ i_k \neq j_k} (-1)^{i_k} = 0 \tag{43}$$

for all I, J such that $|I\rangle\langle J|$ appears with nonzero coefficient in (42), and therefore (35) is zero.

For (36), we have

$$\sum_{k,\ell=1}^{n}(\rho_{I_k,J}-\rho_{I,J_\ell})=\sum_{k,\ell}((-1)^{\mathrm{wt}I_k}c_{I_k^cJ}-(-1)^{\mathrm{wt}I}c_{I^cJ_\ell}) \tag{44}$$

$$=(-1)^{(\mathrm{wt}I+1)}\sum_{k,\ell}(c_{I_k^cJ}+c_{I^cJ_\ell}). \tag{45}$$

The last expression is (a sign times) the coefficient of $|I^cJ\rangle$ in the expansion of $\left(\sum_{k=1}^{2n}C^{(k)}\right)|\mathcal{D}\rangle$), and so this quantity is zero (by (36)) because $|\mathcal{D}\rangle$ is a product of singlets. We conclude that (36) is zero for all I,J.

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