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The Birkhoff theorem for unitary matrices of arbitrary dimensions

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Abstract

It was shown recently that Birkhoff's theorem for doubly stochastic matrices can be extended to unitary matrices with equal line sums whenever the dimension of the matrices is prime. We prove a generalization of the Birkhoff theorem for unitary matrices with equal line sums for arbitrary dimension.

Keywords: Birkhoff's Theorem, Doubly Stochastic Matrix, Unitary Matrix, Irreducible Representation.

1. Introduction

Let M be an arbitrary $n \times n$ doubly-stochastic matrix. Hence, each matrix entry M_{jk} is a real number satisfying $0 \leq M_{jk} \leq 1$ and each line sum, both $\sum_j M_{jk}$ and $\sum_k M_{jk}$ equal 1. Then, the Birkhoff theorem [1] tells us that M can be written as a weighted sum of the $n!$ permutation matrices P_m of

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dimension n:

$$M = \sum_m c_m P_m \qquad (1)$$

such that all coefficients c_m are real and satisfy $0 \le c_m \le 1$ and $\sum_m c_m = 1$.

Let U be an arbitrary $n \times n$ unitary matrix, such that each line sum equals 1, i.e. $\sum_j U_{jk} = 1$ and $\sum_k U_{jk} = 1$. Then, De Vos and De Baerdemacker [2] conjectured that U can be written as a weighted sum of the $n!$ permutation matrices P_m of dimension n:

$$U = \sum_m c_m P_m \qquad (2)$$

such that all coefficients c_m are complex and satisfy both $\sum_m c_m = 1$ and $\sum_m |c_m|^2 = 1$. They proved this fact for the case of prime n. In the present paper we demonstrate that the conjecture, which we will refer to as "Conjecture 1", is also valid for composite n.

Before investigating the mathematics of the proof of Conjecture 1, we stress here three important differences between the 'classical' Birkhoff theorem and the present 'unitary' Birkhoff theorem:

- Whereas the $n \times n$ doubly stochastic matrices form an $(n-1)^2$-dimensional semigroup, the $n \times n$ unit-linesum unitary matrices form an $(n-1)^2$-dimensional group, isomorphic to the unitary group $U(n-1)$ and denoted $XU(n)$ [3].

- The unitary theorem is 'stricter' than the classical theorem, in the sense that $\sum_m |c_m|^2 = 1$ implies $0 \le |c_m| \le 1$ for all m, whereas $0 \le |c_m| \le 1$ for all m does not necessarily imply $\sum_m |c_m|^2 = 1$.

- Let $X(n)$ be the $2(n-1)^2$-dimensional group of all invertible $n \times n$ matrices with complex entries and all line sums equal to 1. The $(n-1)^2$-dimensional group $XU(n)$ is a compact subgroup of $X(n)$. Also the $(n-1)^2$-dimensional semigroup $DS(n)$ of $n \times n$ doubly stochastic matrices resides within $X(n)$. The intersection of the two subsets $XU(n)$ and $DS(n)$ consists of the finite (and thus 0-dimensional) group of $n \times n$ permutation matrices. Proof is in Appendix A. Let P and Q be two arbitrary $n \times n$ permutation matrices. The classical Birkhoff interpolation $(1-c)P + cQ$ with c real and $0 \le c \le 1$ is a line segment in the $(n-1)^2$-dimensional space of $DS(n)$, constituting an edge of the

so-called Birkhoff polytope [4]. In contrast, the quantum Birkhoff interpolation $(1 - c)P + cQ$ with c complex and $|c|^2 + |1 - c|^2 = 1$ is a closed line in the compact $(n-1)^2$-dimensional space of $XU(n)$. The line segment and the closed curve have only the points P and Q in common. This also implies that the classical Birkhoff theorem is not a corollary of the unitary Birkhoff theorem.

The following sections are devoted to the proof and discussion of Conjecture 1 on the unitary Birkhoff theorem. Section 2 recapitulates necessary basic ideas from representation theory, and sections 3 & 4 present the proof of Conjecture 1. Sections 3 and 4 are different in the sense that the former gives an existence proof, whereas the latter presents an explicit construction based on the proof. We conclude the paper with a couple of examples in section 5, and give our conclusions in section 6.

2. Schur decomposition of the permutation matrices

The set of permutation matrices $\{P_\sigma | \sigma \in S_n\}$ forms a reducible representation of S_n. It is straightforward to show that it decomposes into a direct sum of the trivial and standard representation,

$$P = D^{(0)} \oplus D^{(s)}, \tag{3}$$

by means of a similarity transformation with the n-dimensional Fourier matrix F_n. The permutation matrices P_σ form a discrete subgroup of $XU(n)$, and can therefore be brought into block diagonal form by means of [5]

$$F_n^\dagger P_\sigma F_n = \begin{pmatrix} 1 & 0 \\ 0 & D^{(s)}(\sigma) \end{pmatrix}, \tag{4}$$

with the trivial representation $D^{(0)}(\sigma) = 1$ ($\forall \sigma \in S_n$) on the upper-left block, and an $(n-1)$-dimensional representation $D^{(s)}$ on the lower-right block. The latter representation can be identified with the so-called *standard* (irreducible) representation for three reasons. First, the representation is faithful, because the set of permutation matrices forms a faithful representation and F_n is unitary. Second, the representation is irreducible thanks to the orthogonality theorem on the characters of irreducible representations (see Appendix B) [6]. Third, the characters of the irrep depend on the number of invariant points in the permutation ($\sigma(k) = k$), typical for the standard

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representation. As an example, we explicitly construct the standard representation of S_3 by means of the formula in eq. (4). The permutation matrices $\{P_\sigma\}$ in S_3 are given by

$$P_0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad P_{(123)} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad P_{(132)} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \quad (5)$$

$$P_{(12)} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad P_{(13)} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad P_{(23)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

and the Fourier transform F_3 is given by (with $\omega^3 = 1$)

$$F_3 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 & 1 \\ 1 & \omega & \omega^2 \\ 1 & \omega^2 & \omega \end{pmatrix}, \quad (6)$$

so the standard representation becomes

$$D^{(s)}(0) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad D^{(s)}(123) = \begin{pmatrix} \omega^2 & 0 \\ 0 & \omega \end{pmatrix}, \quad D^{(s)}(132) = \begin{pmatrix} \omega & 0 \\ 0 & \omega^2 \end{pmatrix}$$

$$D^{(s)}(12) = \begin{pmatrix} 0 & \omega^2 \\ \omega & 0 \end{pmatrix}, \quad D^{(s)}(13) = \begin{pmatrix} 0 & \omega \\ \omega^2 & 0 \end{pmatrix}, \quad D^{(s)}(23) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

$$(7)$$

Note that the characters of the standard representation indeed correspond with the character table of S_3 (see table 1).

	(1^3)	$(2,1)$	(3)
$D^{(0)}$	1	1	1
$D^{(-)}$	1	−1	1
$D^{(s)}$	2	0	−1

Table 1: Character table of S_3 [6]. The conjugacy classes are labeled by their Young tableaux, and the irreps are the trivial irrep $D^{(0)}$, the sign irrep $D^{(-)}$ and the standard irrep $D^{(s)}$.

3. Birkhoff's theorem for unitary matrices

The existence proof of the unitary Birkhoff theorem is a corollary of two theorems, the first being provided by some of us [2] and the second by Klappenecker & Rötteler [7].

Theorem 1 (De Vos & De Baerdemacker [2]). *If a matrix belongs to $XU(n)$, then it can be written as a weighted sum of permutation matrices with the sum of the weights equal to 1.*

This theorem was proven by induction in [2]. Before phrasing the second theorem, we need to introduce the concept of a *group-circulant* matrix of a finite group G of order d, associated to a vector $|c\rangle \in \mathbb{C}^d$. Assume a one-to-one mapping between the elements $g \in G$ and the components c_g of the vector $|c\rangle$, then the $(d \times d)$-matrix

$$\mathrm{circ}_G(|c\rangle) := (c_{g^{-1}h})_{g,h \in G} \tag{8}$$

is called the group-circulant for the group G, associated to $|c\rangle$. The second theorem now states

Theorem 2 (Klappenecker & Rötteler [7]). *Let D be a matrix representation of a finite group G $(g \to D(g))$. If a unitary matrix A can be expressed as linear combination*

$$A = \sum_{g \in G} c_g D(g), \qquad c_g \in \mathbb{C}, \tag{9}$$

then the coefficients c_g of the vector $|c\rangle$ can be chosen such that the associated group-circulant matrix is also unitary.

These two theorems essentially prove the Birkhoff theorem for unitary matrices of arbitrary dimensions. Indeed, the permutation matrices form a matrix representation of the symmetric group for any dimension. Theorem 1 ensures that any matrix $X \in XU(n)$ can be expressed as a linear combination of the permutation matrices

$$X = \sum_{\sigma \in S_n} c_\sigma P_\sigma, \tag{10}$$

so the two prerequisites of Theorem 2 are met. Therefore, one can choose the vector $|c\rangle$ such that its associated group circulant matrix $\mathrm{circ}_{S_n}(|c\rangle)$ is

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unitary. More specific, this implies that $|c\rangle$ can be chosen such that

$$\sum_{\sigma \in S_n} |c_\sigma|^2 = 1. \tag{11}$$

This essentially proves our Conjecture 1 on the Birkhoff theorem for unitary matrices. However, we will go one step further and present explicit expressions for the c_σ coefficients in Theorem 3 in the following section.

Before presenting Theorem 3, it is useful to recapitulate the key concepts in the proof of Theorem 2 by Klappenecker & Rötteler [7]. The proof relies entirely on the Schur orthonormality of the irreps of finite groups. Just like in the previous paper [2], it is most instructive to consider the $n = 3$ example before illustrating the general case. The claim is that any $X \in \mathrm{XU}(3)$ can be written as

$$X = \sum_{\sigma \in S_3} c_\sigma P_\sigma. \tag{12}$$

with $\sum_{\sigma \in S_3} c_\sigma = 1$ and $\sum_{\sigma \in S_3} |c_\sigma|^2 = 1$. Performing a similarity transformation with the F_3 Fourier matrix of eq. (6) on the lhs and rhs of eq. (12) gives rise to

$$\begin{pmatrix} 1 & 0 \\ 0 & U^{(s)} \end{pmatrix} = \sum_{\sigma \in S_3} c_\sigma \begin{pmatrix} 1 & 0 \\ 0 & D^{(s)}(\sigma) \end{pmatrix}, \tag{13}$$

with $U^{(s)} \in U(2)$, and the standard representation $D^{(s)}(\sigma)$ of S_3 given by the matrices (7). By equating all matrix elements explicitly, this gives rise to the following set of (five) equations

$$1 = c_0 + c_{(123)} + c_{(132)} + c_{(12)} + c_{(13)} + c_{(23)}, \tag{14}$$

$$U_{11}^{(s)} = c_0 + \omega^2 c_{(123)} + \omega c_{(132)}, \tag{15}$$

$$U_{22}^{(s)} = c_0 + \omega c_{(123)} + \omega^2 c_{(132)}, \tag{16}$$

$$U_{12}^{(s)} = c_{(23)} + \omega^2 c_{(12)} + \omega c_{(13)}, \tag{17}$$

$$U_{21}^{(s)} = c_{(23)} + \omega c_{(12)} + \omega^2 c_{(13)}. \tag{18}$$

Note that the first equation $1 = \sum_\sigma c_\sigma$ confirms Theorem 1. The linear set of equations contains six variables, so one needs one additional equation to find a closed solution. Remark that the sign representation $D^{(-)}(\sigma)$ is the only irrep missing in eq. (13). Indeed, one can augment the 3×3 matrix

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equality to a 4×4 matrix equality by adding the sign representation $D^{(-)}(\sigma)$ on the diagonal

$$
\begin{pmatrix} 1 & 0 & 0 \\ 0 & U^{(s)} & 0 \\ 0 & 0 & e^{i\phi} \end{pmatrix} = \sum_{\sigma \in S_3} c_\sigma \begin{pmatrix} D^{(0)}(\sigma) & 0 & 0 \\ 0 & D^{(s)}(\sigma) & 0 \\ 0 & 0 & D^{(-)}(\sigma) \end{pmatrix}, \qquad (19)
$$

where we have used that $1 = D^{(0)}(\sigma)$ for all σ, and $e^{i\phi} \in U(1)$ is an arbitrary 1×1 unitary matrix. This extra equation reads

$$
e^{i\phi} = c_0 + c_{(123)} + c_{(132)} - c_{(12)} - c_{(13)} - c_{(23)}. \qquad (20)
$$

Solving eqs. (14-18,20) for c_σ, we obtain

$$
c_0 = \tfrac{1}{3}[\tfrac{1}{2}(1 + e^{i\phi}) + U^{(s)}_{11} + U^{(s)}_{22}] \qquad (21)
$$

$$
c_{(123)} = \tfrac{1}{3}[\tfrac{1}{2}(1 + e^{i\phi}) + \omega U^{(s)}_{11} + \omega^2 U^{(s)}_{22}] \qquad (22)
$$

$$
c_{(132)} = \tfrac{1}{3}[\tfrac{1}{2}(1 + e^{i\phi}) + \omega^2 U^{(s)}_{11} + \omega U^{(s)}_{22}] \qquad (23)
$$

$$
c_{(23)} = \tfrac{1}{3}[\tfrac{1}{2}(1 - e^{i\phi}) + U^{(s)}_{12} + U^{(s)}_{21}] \qquad (24)
$$

$$
c_{(12)} = \tfrac{1}{3}[\tfrac{1}{2}(1 - e^{i\phi}) + \omega U^{(s)}_{12} + \omega^2 U^{(s)}_{21}] \qquad (25)
$$

$$
c_{(13)} = \tfrac{1}{3}[\tfrac{1}{2}(1 - e^{i\phi}) + \omega^2 U^{(s)}_{12} + \omega U^{(s)}_{21}]. \qquad (26)
$$

Taking into account that $U^{(s)}$ is unitary, it is straightforward to verify that $\sum_\sigma |c_\sigma|^2 = 1$, which again proves the unitary Birkhoff theorem for $n = 3$. Note that the choice $\phi = 0$ coincides exactly with the choice $p = 1$ in [2]. More generally, the correspondence between the present solution and the one presented in [2], is $p = \tfrac{1}{2}(1 + e^{i\phi})$, coinciding with the observation that p had to lie on a circle in the complex plane with radius $\tfrac{1}{2}$ and center $\tfrac{1}{2}$.

For the proof of the general case, we proceed in a similar manner. Theorem 1 states that any $X \in \mathrm{XU}(n)$ can be written as

$$
X = \sum_{\sigma \in S_n} c_\sigma P_\sigma. \qquad (27)
$$

Applying the similarity transform with the F_n Fourier transform, we obtain

$$
\begin{pmatrix} 1 & 0 \\ 0 & U^{(s)} \end{pmatrix} = \sum_{\sigma \in S_n} c_\sigma \begin{pmatrix} D^{(0)}(\sigma) & 0 \\ 0 & D^{(s)}(\sigma) \end{pmatrix}, \qquad (28)
$$

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with $U^{(s)} \in \mathrm{U}(n-1)$. This results in a set of $(n-1)^2 + 1$ equations with $n!$ variables c_σ, so we need $n! - (n-1)^2 - 1$ more equations to find a closed solution via linear algebra. Now, one can augment the $n \times n$ matrix with all other possible irreps $D^{(\nu)}$ of S_n on the (block) diagonal in the rhs summation, and arbitrary n_ν dimensional unitary matrices $U^{(\nu)} \in \mathrm{U}(n_\nu)$ on the corresponding (block) diagonal parts in the lhs, with n_ν the dimension of irrep $D^{(\nu)}$

$$
\begin{pmatrix} 1 & & & \\ & U^{(s)} & & \\ & & U^{(2)} & \\ & & & \ddots \end{pmatrix} = \sum_{\sigma \in S_n} c_\sigma \begin{pmatrix} D^{(0)}(\sigma) & & & \\ & D^{(s)}(\sigma) & & \\ & & D^{(2)}(\sigma) & \\ & & & \ddots \end{pmatrix}.
$$
(29)

The resulting matrix has dimension $d(n) = \sum_{\nu=0}^{k-1} n_\nu$ with k the number of conjugacy classes of S_n, i.e., the number of partitions of integer n [8]. The number $d(n)$ equals the number of involutions on n objects and is tabulated in [9]. The augmented matrices in the rhs summation in (29) form again a reducible representation, known as the *regular* representation [10]. We will label the standard representation $D^{(s)} = D^{(1)}$ from now on for the sake of notation.

The key observation is that there are as many irrep matrix elements $D_{ij}^{(\nu)}(\tau)$ ($\nu = 0, \ldots, k-1$ & $i, j = 1, \ldots n_\nu$) for any $\tau \in S_n$ as there are group elements σ in S_n. Therefore, $D_{ij}^{(\nu)}(\sigma)$ can be regarded as a matrix element of an $n! \times n!$ matrix D with indices $\{\nu, i, j\}$ for the "rows" and σ for the "columns". Due to Schur's orthogonality theorems,

$$
n_\nu \sum_{\sigma \in S_n} D_{ij}^{(\nu)*}(\sigma) D_{lm}^{(\mu)}(\sigma) = n! \delta_{\mu\nu} \delta_{il} \delta_{jm}
$$
(30)

$$
\sum_{\nu=0}^{k-1} n_\nu \sum_{ij=1}^{n_\nu} D_{ij}^{(\nu)*}(\sigma) D_{ij}^{(\nu)}(\tau) = n! \delta_{\sigma\tau}
$$
(31)

it follows directly that the (rescaled) matrix $\tilde{D}$ is a unitary matrix, with $\tilde{D}_{ij}^{(\nu)}(\sigma) = \sqrt{\frac{n_\nu}{n!}} D_{ij}^{(\nu)}(\sigma)$. This means that the set of $n!$ equations

$$
U_{ij}^{(\nu)} = \sum_{\sigma \in S_n} c_\sigma D_{ij}^{(\nu)}(\sigma), \quad \forall \nu, i, j,
$$
(32)

extracted from the block diagonals of eq. (29) can be solved uniquely by inverting the non-singular matrix D. This is exactly what has been done in

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Theorem 3 in the following section to construct explicit expressions for the coefficients c_σ in the Birkhoff summation.

4. Explicit decomposition

Theorem 3. *Every matrix $X \in XU(n)$ can be written as a weighted sum of permutation matrices*

$$X = \sum_{\sigma \in S_n} c_\sigma P_\sigma, \tag{33}$$

with the coefficients c_σ given by

$$c_\sigma = \frac{1}{n!} \sum_\nu n_\nu \sum_{ij=1}^{n_\nu} D_{ij}^{(\nu)*}(\sigma) U_{ij}^{(\nu)}, \tag{34}$$

$$= \frac{1}{n!} \sum_\nu n_\nu \operatorname{Tr}(D^{(\nu)\dagger}(\sigma) U^{(\nu)}) \tag{35}$$

where the sum ν runs over all possible irreps $D^{(\nu)}$ of S_n, n_ν is the dimension of $D^{(\nu)}$, and $U^{(\nu)} \in U(n_\nu)$ is a unitary matrix associated to $D^{(\nu)}$. All unitary matrices $U^{(\nu)}$ can be chosen arbitrarily, with the exception of $U^{(0)} = 1 \in U(1)$ and $U^{(1)} = U^{(s)} \in U(n-1)$ associated to respectively the trivial and standard representation, which are found by

$$F_n^\dagger X F_n = \begin{pmatrix} U^{(0)} & 0 \\ 0 & U^{(s)} \end{pmatrix}. \tag{36}$$

In addition, the sum of the moduli squared equals 1

$$\sum_{\sigma \in S_n} |c_\sigma|^2 = 1. \tag{37}$$

The proof goes by straightforward application of Shur's orthogonality relations. First, we verify that eq. (36) holds when the c_σ coefficients are taken as in expression (35) (from which X follows directly by means of the similarity transform $F_n(F_n^\dagger X F_n)F_n^\dagger = X$.). Because of the Schur decomposition (4) of the permutation matrices P_σ, $F_n^\dagger X F_n$ is also block diagonal. We first investigate the upper left matrix element

$$(F_n^\dagger X F_n)_{11} = \sum_{\sigma \in S_n} c_\sigma (F_n^\dagger P_\sigma F_n)_{11} = \sum_{\sigma \in S_n} c_\sigma D_{11}^{(0)}(\sigma) \tag{38}$$

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in which we prefer to keep the explicit notation for the trivial representation $D_{11}^{(0)}(\sigma) = 1$ in the Schur decomposition of the permutation matrices (4). We now insert the explicit expression (35) for c_σ in (38) and rearrange the summation

$$(F_n^\dagger X F_n)_{11} = \frac{1}{n!} \sum_\nu n_\nu \sum_{ij=1}^{n_\nu} U_{ij}^{(\nu)} \sum_{\sigma \in S_n} D_{ij}^{(\nu)*}(\sigma) D_{11}^{(0)}(\sigma) = U_{11}^{(0)}, \qquad (39)$$

where the Schur orthogonality relation (30) has been used in the last step. Because $U^{(0)} \equiv 1$ in the present theorem, we get that the upper left element of $F_n^\dagger X F_n$ equals 1. The other matrix elements can be obtained analogously from Schur's orthogonality relation (30)

$$(F_n^\dagger X F_n)_{lm} = U_{l-1,m-1}^{(1)} \equiv U_{l-1,m-1}^{(s)}, \qquad \forall l, m = 2, \ldots, n. \qquad (40)$$

The compactness of the c_σ coefficients (37) can also be proven similarly

$$\sum_{\sigma \in S_n} |c_\sigma|^2 = \sum_{\sigma \in S_n} c_\sigma c_\sigma^* \qquad (41)$$

$$= \frac{1}{n!^2} \sum_{\nu\mu} n_\nu n_\mu \sum_{ij=1}^{n_\nu} \sum_{lm=1}^{n_\mu} U_{ij}^{(\nu)} U_{lm}^{(\mu)*} \sum_{\sigma \in S_n} D_{ij}^{(\nu)*}(\sigma) D_{lm}^{(\mu)}(\sigma) \qquad (42)$$

$$= \frac{1}{n!} \sum_\nu n_\nu \sum_{ij=1}^{n_\nu} U_{ij}^{(\nu)} U_{ij}^{(\nu)*} \qquad (43)$$

$$= \frac{1}{n!} \sum_\nu n_\nu \operatorname{Tr}(U^{(\nu)} U^{(\nu)\dagger}). \qquad (44)$$

Because $U^{(\nu)}$ are unitary, we have that $\operatorname{Tr}(U^{(\nu)} U^{(\nu)\dagger}) = n_\nu$, so

$$\sum_{\sigma \in S_n} |c_\sigma|^2 = \frac{1}{n!} \sum_\nu n_\nu^2 = 1. \qquad (45)$$

This completes the proof.

Theorem 3 allows for a large freedom of choice, associated with all unitary matrices $U^{(\nu)}$ ($\nu > 1$) that can be chosen arbitrarily. As an example, we investigate the choice $U^{(\nu)}$ (for $\nu > 1$) equal to $D^{(\nu)}(\tau)$, where τ is one

particular permutation, i.e. a particular member of S_n. Eq. (35) thus becomes

$$c_\sigma = \frac{1}{n!} \sum_{\nu=0}^{k-1} n_\nu \text{Tr} \left(D^{(\nu)}(\sigma)^\dagger D^{(\nu)}(\tau) \right)$$
$$- \frac{n_1}{n!} \text{Tr} \left(D^{(1)}(\sigma)^\dagger D^{(1)}(\tau) \right) + \frac{n_1}{n!} \text{Tr} \left(D^{(1)}(\sigma)^\dagger U^{(1)} \right). \qquad (46)$$

Taking into account that $n_1 = n - 1$, $D^{(1)}(\sigma)^\dagger = D^{(1)}(\sigma^{-1})$, and that the first term in the equation is Shur's orthogonality relation, we obtain

$$c_\sigma = \delta_{\sigma\tau} - \frac{n-1}{n!} \chi^{(1)}(\sigma^{-1}\tau) + \frac{n-1}{n!} \text{Tr} \left(D^{(1)}(\sigma^{-1})U^{(1)} \right). \qquad (47)$$

For instance, substituting $n = 3$ and $\tau = (0)$ the identity, we immediately recover (19-24) with $\phi = 0$.

Note that in contrast to eq. (35), only the standard representation $D^{(s)}$ occurs in the expression (47) for the c_σ coefficient. From a practical point of view, this is very convenient because the standard representation can quickly be obtained by reducing the n-dimensional permutation representation (4). Hence, no other representations need to be constructed from other means.

If $n > 3$, then another elegant choice is possible. Again, we choose $U^{(\nu)} = D^{(\nu)}(\tau)$, however, now with *two* exceptions: both $U^{(s)} = U$ and $U^{(a)} = U$. Here, $U^{(s)}$ corresponds, in (29), with the standard representation $D^{(s)}$ of dimension $n - 1$, whereas $U^{(a)}$ corresponds with the other $(n-1)$-dimensional representation $D^{(a)}$ in (29), which we will call the 'anti-standard' representation. The anti-standard representation of S_n consists of the same matrices as the standard representation, except for a minus sign in case of an odd permutation[1]. Now, eq. (35) becomes

$$c_\sigma = \delta_{\sigma\tau} - \frac{n-1}{n!}\chi^{(s)}(\sigma^{-1}\tau) + \frac{n-1}{n!}\text{Tr}\left(D^{(s)}(\sigma^{-1})U^{(1)} \right)$$
$$- \frac{n-1}{n!}\chi^{(a)}(\sigma^{-1}\tau) + \frac{n-1}{n!}\text{Tr}\left(D^{(a)}(\sigma^{-1})U^{(1)} \right). \qquad (48)$$

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[1]Also for $n = 2$ and $n = 3$ an anti-standard representation exists. However, for $n = 2$, the anti-standard representation equals the trivial representation and for $n = 3$, the anti-standard representation is equivalent to the standard representation:

$$D^{(a)}(\sigma) = \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} D^{(s)}(\sigma) \begin{pmatrix} 1 & \\ & -1 \end{pmatrix}.$$

Restricting ourselves to the obvious choice $\tau = (0)$, we obtain,

$$c_\sigma = \begin{cases} \delta_{\sigma 0} - 2\,\frac{n-1}{n!}\,\chi^{(s)}(\sigma) + 2\,\frac{n-1}{n!}\,\mathrm{Tr}\left(D^{(s)}(\sigma^{-1})U\right), & \sigma \text{ even} \\ 0, & \sigma \text{ odd.} \end{cases} \tag{49}$$

Yet another choice is $U^{(s)} = U$ and $U^{(a)} = -U$. It yields

$$c_\sigma = \delta_{\sigma 0} - 2\,\frac{n-1}{n!}\,\chi^{(s)}(\sigma) \tag{50}$$

for even σ and

$$c_\sigma = 2\,\frac{n-1}{n!}\,\mathrm{Tr}\left(D^{(s)}(\sigma^{-1})U\right) \tag{51}$$

for odd σ. Again, only the standard representation $D^{(s)}$ is required.

5. Examples

We now present two examples for the non-prime $n = 4$ case. In the framework of quantum multiports [11], it is important to synthesize $n \times n$ matrices with all entries having the same modulus (and thus modulus equal to $1/\sqrt{n}$). As an example, we consider the XU(4) matrix

$$X = \frac{1}{2}\begin{pmatrix} 1 & -i & 1 & i \\ 1 & 1 & -1 & 1 \\ 1 & i & 1 & -i \\ -1 & 1 & 1 & 1 \end{pmatrix}. \tag{52}$$

Up to phase changes, it equals the 4×4 Fourier transform. Indeed:

$$\begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix} X \begin{pmatrix} 1 & & & \\ & i & & \\ & & 1 & \\ & & & -i \end{pmatrix} = F_4 . \tag{53}$$

Applying (49) to X yields, besides the twelve zero coefficients for the odd permutation matrices, the following weights for the twelve even permutation matrices:

$$\frac{1}{8}\left\{4, -1-i, 1+i, 2-2i, -1-i, -1-i, 1+i, -1-i, 4, 1+i, 1+i, -2+2i\right\}, \tag{54}$$

satisfying $\sum_\sigma c_\sigma = \sum_\sigma |c_\sigma|^2 = 1$.

Because a 4×4 permutation matrix is also an $XU(4)$ matrix, we can e.g. apply (49) to the odd permutation matrix

$$
\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{pmatrix} ,
\tag{55}
$$

resulting in a Birkhoff decomposition with even permutation matrices with weights

$$
\frac{1}{4} \, \{2, 1, 1, 2, -1, -1, -1, 1, 0, -1, 1, 0\} .
\tag{56}
$$

Again we have $\sum_\sigma c_\sigma = \sum_\sigma |c_\sigma|^2 = 1$. It is remarkable that, for $n > 3$, one can decompose any permutation, either even or odd, into a sum of only even permutation matrices.

6. Conclusion

Recently, we proved a Birkhoff theorem for unitary matrices of prime dimension [2]. In the present manuscript, we complete the proof of the theorem for unitary matrices of arbitrary dimension n. The proof is based on a theorem by Klappenecker and Rötteler [7], employing the Schur orthonormality of the representations of the permutation group S_n. Furthermore, we present an explicit construction of the weight coefficients in the Birkhoff decomposition. There is a freedom of choice in the explicit construction, allowing one to express the coefficients exclusively in terms of the known $(n-1)$-dimensional standard representation. Remarkably, this leads to a decomposition of any unitary matrix, for $n > 3$, into a weighted sum of only even permutation matrices. It would be interesting to explore the freedom of choice inherent in the procedure in order to obtain different and possibly shorter Birkhoff decompositions.

Acknowledgements

Appendix A. Unitary doubly stochastic matrices

Theorem 4. *The only unitary doubly stochastic matrices are the permutation matrices.*

Proof. Let M be an $n \times n$ matrix that is simultaneously member of $\mathrm{XU}(n)$ and $\mathrm{DS}(n)$. Because $M \in \mathrm{DS}(n)$, all its entries are either zero or positive. Every row of M contains at least one non-zero entry (because otherwise the related row sum would equal 0). The row cannot contain more than one non-zero entry. Indeed, suppose the ath row contains two positive entries M_{ab} and M_{ac} ($b \neq c$). Then the sum $\sum_j M_{jb} M_{jc}$ contains at least one positive term, i.e. $M_{ab} M_{ac}$. All the other $n - 1$ terms in the summation are either zero or positive, so we have $\sum_j M_{jb} M_{jc} > 0$.

Because M is a unitary matrix, we also have that $\sum_j (M^\dagger)_{kj} M_{jl} = \delta_{kl}$, or $\sum_j M_{jb} M_{jc} = 0$, which contradicts the previous paragraph.

Hence, every row of M contains exactly one non-zero entry, and so does every column. Because all line sums are equal to 1, these non-zero entries necessarily equal 1. We conclude that M is a permutation matrix.

Appendix B. Reducibility of the permutation matrices

The orthogonality theorem on the characters of irreducible representations (see section 3-16. in [6]) states that a representation $D^{(\nu)}$ is irreducible iff the sum of all characters squared $|\chi^\nu(\sigma)|^2$ over all possible group elements equals the order of the group. For the symmetric group S_n, this becomes

$$\sum_{\sigma \in S_n} |\chi^{(\nu)}(\sigma)|^2 = n!. \tag{B.1}$$

So, if this relation holds for the representation $D^{(s)}$ in eq. (4), it is irreducible. The character

$$\chi^{(s)}(\sigma) = \mathrm{Tr}[D^{(s)}(\sigma)] \tag{B.2}$$

can be obtained for each permutation σ explicitly. We indeed have that

$$\mathrm{Tr}\left[D^{(s)}(\sigma)\right] = \mathrm{Tr}\left(F^\dagger P_\sigma F\right) - 1, \tag{B.3}$$

because $D^{(s)}(\sigma)$ is obtained from $F^\dagger P_\sigma F$ by deleting its first row and first column. Because a trace is similarity-invariant, this yields

$$\chi^{(s)}(\sigma) = \mathrm{Tr}\left(P_\sigma\right) - 1. \tag{B.4}$$

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As a result, the characters depend on the number of ones on the diagonal in the original matrix P_σ only, in a way typical for the standard representation. Thus, the characters $\chi^{(s)}$ are the rational integers ranging from -1 to $n-1$, except $n-2$. The character formula (B.1) becomes

$$\sum_{\sigma \in S_n} |\chi^{(s)}(\sigma)|^2 = \sum_{\sigma \in S_n} \left(\sum_{l=1}^{n} \delta_{l\sigma(l)} - 1 \right) \left(\sum_{k=1}^{n} \delta_{k\sigma(k)} - 1 \right) \tag{B.5}$$

$$= \sum_{l=1}^{n} \sum_{k=1}^{n} \sum_{\sigma \in S_n} \delta_{l\sigma(l)}\delta_{k\sigma(k)} - 2 \sum_{k=1}^{n} \sum_{\sigma \in S_n} \delta_{k\sigma(k)} + n!. \tag{B.6}$$

Taking into account that $\delta^2_{k\sigma(k)} = \delta_{k\sigma(k)}$, this can be slightly rewritten as

$$\sum_{\sigma \in S_n} |\chi^{(s)}(\sigma)|^2 = \sum_{l=1}^{n} \sum_{k \neq l} \sum_{\sigma \in S_n} \delta_{l\sigma(l)}\delta_{k\sigma(k)} - \sum_{k=1}^{n} \sum_{\sigma \in S_n} \delta_{k\sigma(k)} + n!. \tag{B.7}$$

Both sums are quite straightforward to reason. There are exactly $(n-1)!$ permutations σ in S_n that leave k invariant $\sigma(k) = k$, leading to

$$\sum_{k=1}^{n} \sum_{\sigma \in S_n} \delta_{k\sigma(k)} = \sum_{k=1}^{n} (n-1)! = n!. \tag{B.8}$$

Similarly, there are exactly $(n-2)!$ permutations σ in S_n that leave k and $l(\neq k)$ invariant, leading to

$$\sum_{l=1}^{n} \sum_{k \neq l} \sum_{\sigma \in S_n} \delta_{l\sigma(l)}\delta_{k\sigma(k)} = \sum_{l=1}^{n} \sum_{k \neq l} (n-2)! = n!. \tag{B.9}$$

As a result, the character orthogonality formula (B.1) becomes

$$\sum_{\sigma \in S_n} |\chi^{(s)}(\sigma)|^2 = n! - n! + n! \equiv n!, \tag{B.10}$$

pointing out that the representation $D^{(s)}$ is indeed irreducible.

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