



Defect of a unitary matrix

Wojciech Tadej^{a,*}, Karol Życzkowski^{b,c}

^a Faculty of Mathematics and Natural Sciences, College of Sciences, Cardinal Stefan Wyszyński University, Warsaw, Poland

^b Institute of Physics, Jagiellonian University, Kraków, Poland

^c Center for Theoretical Physics, Polish Academy of Sciences, Warsaw, Poland

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Abstract

We analyze properties of a map f sending a unitary matrix U of size N into a doubly stochastic matrix $B = f(U)$ defined by $B_{i,j} = |U_{i,j}|^2$. For any U we define its *defect*, determined by the dimension of the image $Df(\mathbf{T}_U\mathcal{U})$ of the space $\mathbf{T}_U\mathcal{U}$ tangent to the manifold of unitary matrices \mathcal{U} at U under the tangent map Df corresponding to f . The defect of U equal to zero for a generic unitary matrix, gives an upper bound for the dimension of a smooth orbit (a manifold) stemming from U of inequivalent unitary matrices mapped into the same doubly stochastic matrix $B = f(U)$. We demonstrate several properties of the defect and prove an explicit formula for the defect of the Fourier matrix F_N of size N . In this way we obtain an upper bound for the dimension of a smooth orbit of inequivalent unitary complex Hadamard matrices stemming from F_N . It is equal to zero iff N is prime and coincides with the dimension of the known orbits if N is a power of a prime. Two constructions of these orbits are presented at the end of this work.

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1. Introduction

Consider the set \mathcal{U} of unitary matrices of finite size N . For any unitary U we define a matrix $B = f(U)$ with non-negative entries

* Corresponding author.

E-mail addresses: wtadej@wp.pl (W. Tadej), karol@taty.if.uj.edu.pl (K. Życzkowski).

$$B_{i,j} = |U_{i,j}|^2. \quad (1)$$

From the unitarity condition, $UU^* = \mathbb{1}$, it follows that the resulting matrix B is bistochastic (also called *doubly stochastic*), since the sum of elements in each of its columns or rows is equal to unity. A bistochastic matrix B for which there exists a unitary (an orthogonal) U satisfying (1) is called *unistochastic* (*orthostochastic*). For $N = 2$ all bistochastic matrices are unistochastic, even orthostochastic, but for $N \geq 3$ it is no longer the case [1,2].

Our work is motivated by the following problem [3,4].

(*) For a given unitary $U \in \mathcal{U}$ find all other unitary matrices $V \in \mathcal{U}$ such that $f(V) = B = f(U)$.

This rather general question is closely related to several problems in various branches of mathematics and theoretical physics. For instance, taking the Fourier matrix F_N as the unitary U in question we get the flat bistochastic matrix, $B = J_N$ with $[J_N]_{i,j} = 1/N$, so the above question reduces to the problem of finding all unitary¹ complex Hadamard matrices of size N . This issue is related to construction of some $*$ -subalgebras in finite von Neumann algebras [6,7,8], analyzing bi-unimodular sequences or finding cyclic n -roots [9,10] and equiangular lines [11]. The search for complex Hadamard matrices [8,12] is also motivated by the theory of quantum information processing [13–15].

Furthermore, the general issue of specifying all unitary matrices such that their squared moduli give a fixed bistochastic matrix was intensively studied by high energy physicists investigating the parity violation and analyzing the Cabibbo–Kobayashi–Maskawa matrices [16,17,18]. On the other hand, relation (1) is relevant to investigation of the semiclassical limit of quantum mechanics: for a given bistochastic B , representing the transition matrix of a Markov chain, one looks for the set of unitary matrices U which lead to the corresponding quantum dynamics [19,20,21].

To investigate problem (*) one uses the notion of *equivalent* unitary matrices [8], which differ by left and right multiplication by diagonal unitary matrices followed by arbitrary permutations of rows and columns. We suppose that for a generic unitary U all solutions of the problem (*) in a neighbourhood of U are equivalent, and we call such U *isolated*. However, for some non-typical unitaries it is not the case. It is therefore natural to ask for the dimension of a smooth orbit, i.e. a manifold, stemming from U , if one exists, of non-equivalent solutions V of problem (*) posed for a given unitary U . The upper bound for this dimension is obtained in this paper by computing the difference between the dimension $(N - 1)^2$ of the minimal affine space \mathcal{B} containing all bistochastic matrices, and the dimension of the image $Df(\mathbf{T}_U \mathcal{U})$ of the space $\mathbf{T}_U \mathcal{U}$, tangent to \mathcal{U} at U , under the tangent map Df . A non-negative integer number resulting from this calculation for a given unitary matrix U will be called its *defect*. We conjectured the defect to be equal to zero for a generic U , as a non-zero defect condition has the form of one additional equation imposed on entries of U . As we have been recently informed, the statement that the set of unitary matrices with a non-zero defect has measure zero within the set of all unitaries follows from an early work by Karabegov [22].

Any non-zero value of the defect may be considered as a kind of quantification of the particular structure of U . For instance, the defect is positive if U is an orthogonal matrix of size $N \geq 3$, if U has a certain *pattern* i.e. some of its entries are equal to zero, or if U has a Kronecker product structure.

¹ We reserve the term ‘complex Hadamard matrix’ for an $N \times N$ complex matrix H satisfying $H^*H = HH^* = N \cdot I_N$ and $\forall i, j |H_{i,j}| = 1$, while $1/\sqrt{N} \cdot H$ is called a ‘unitary complex Hadamard matrix’. Such matrices were called by Craigen ‘unit Hadamard matrices’ [5].

After the definition of the defect was first proposed in our previous work [15], this concept was used in very recent papers [27,28] to characterize complex Hadamard matrices. In this work we prove several properties of the defect, demonstrating its invariance with respect to the equivalence relation. We show that vanishing of the defect of U implies that U is isolated and we find a relation to an analogous ‘span condition’ by Nicoara [24].

The key result of this paper we regard to be an explicit formula for the defect of the Fourier matrix F_N of size N . Equivalent, more transparent forms of this formula were obtained by W. Słomczyński and are proved in Appendix B. The defect vanishes iff N is prime, which implies the earlier statement by Petrescu [25] that the Fourier matrix is isolated if its dimension is a prime number. This in turn implies that the flat bistochastic matrix J_N belongs to the interior of the set of unistochastic matrices [4], if N is prime.

For a composite N the defect of F_N is positive, and it is usually greater than the dimension of *affine Hadamard families* stemming from F_N , introduced in [15]. However, if the size of a matrix is a power of prime, $N = p^k$, the defect and the dimension coincide. So, in this very case, an explicit construction of the defect-dimensional affine family of unitary complex Hadamard matrices stemming from the Fourier matrix is complete. By ‘complete’ we mean that this solution cannot be embedded inside any orbit of inequivalent complex Hadamard matrices of a larger dimension.

This work is organized as follows. In Section 2 the definition of the defect of a unitary matrix is provided. Several properties of the defect are investigated in Section 3. In Section 4 we present some applications of the defect analyzing the condition for a unitary matrix to be isolated and discussing the unistochasticity problem. Section 5 contains derivation of the formula for the defect of the Fourier matrix of an arbitrary size N and a discussion of its special cases. In Section 6 we provide two constructions of the defect-dimensional orbit of unitary complex Hadamard matrices stemming from F_N for N being a power of a prime number. The paper is concluded in Section 7.

We use in the paper the notation $A \circ B$ for the Hadamard product of two matrices, $[A \circ B]_{i,j} = A_{i,j} B_{i,j}$, while $\mathbf{EXP}(A)$ denotes entrywise exponentiation of a matrix, $[\mathbf{EXP}(A)]_{i,j} = \exp(A_{i,j})$. Also, as functions of matrices are used, to avoid doubts about an order of variables, for example when writing Jacobi matrices, we introduce \mathbf{vec} , $\mathbf{vec}_{\mathbb{R}}$, $\mathbf{vec}_{\mathbb{C}}$ notation for appropriate vector forms of each matrix. Such notations make it possible for us to treat manifolds of matrices and their tangent spaces as subsets of \mathbb{R}^k , identified with the set of all real $k \times 1$ column matrices, and avoid more abstract constructions. These and other symbols used are listed and explained in Appendix A.

2. The defect of a unitary matrix

2.1. Definition of the defect

Let $\mathbf{vec}_{\mathbb{R}}(\mathcal{U})$ be a submanifold of \mathbb{R}^{2N^2} representing the set \mathcal{U} of all $N \times N$ unitary matrices (for the notation consult Appendix A). Consider also the $(N - 1)^2$ dimensional minimal hyperplane containing bistochastic matrices $\mathbf{vec}(\mathcal{B}) \subset \mathbb{R}^{N^2}$, and a map $f : \mathbb{R}^{2N^2} \rightarrow \mathbb{R}^{N^2}$, effectively squaring the moduli of the entries of an $N \times N$ complex matrix U :

$$f(\mathbf{vec}_{\mathbb{R}}(U)) = \mathbf{vec}(B), \quad \text{where } B_{i,j} = |U_{i,j}|^2. \tag{2}$$

Next consider the tangent map $Df_{\mathbf{vec}_{\mathbb{R}}(U)} : \mathbb{R}^{2N^2} \rightarrow \mathbb{R}^{N^2}$, realized by the appropriate Jacobi matrix:

$$Df_{\text{vec}_{\mathbb{R}}(U)}(\text{vec}_{\mathbb{R}}(V)) = 2 \cdot [\text{diag}(\text{vec}(\text{Re}(U))) | \text{diag}(\text{vec}(\text{Im}(U)))] \cdot \text{vec}_{\mathbb{R}}(V). \tag{3}$$

Consider also the tangent spaces, the space $\mathbf{T}_U \mathcal{U}$ tangent to $\text{vec}_{\mathbb{R}}(\mathcal{U})$ at $\text{vec}_{\mathbb{R}}(U)$ for some unitary $U \in \mathcal{U}$, and the space $\mathbf{T}_B \mathcal{B}$ tangent to $\text{vec}(\mathcal{B})$ at $\text{vec}(B) = f(\text{vec}_{\mathbb{R}}(U))$, a bistochastic matrix. $\mathbf{T}_U \mathcal{U}$ here and further is understood as the nullspace of the Jacobi matrix of the map $\text{vec}_{\mathbb{R}}(W) \rightarrow \text{vec}_{\mathbb{R}}(W^*W - I)$ calculated at $\text{vec}_{\mathbb{R}}(U)$ (i.e. the kernel of the corresponding tangent map). $\mathbf{T}_B \mathcal{B}$ is the space of all vectors $\text{vec}(G)$ with G being a real $N \times N$ matrix with sums of all entries in each row and column equal to zero, irrespectively of a bistochastic B . It is clear that the image of $\mathbf{T}_U \mathcal{U}$ under $Df_{\text{vec}_{\mathbb{R}}(U)}$ must be contained in $\mathbf{T}_B \mathcal{B}$, so its dimension is not greater than $(N - 1)^2$. It is reduced, with respect to that value, by a number which will be called *defect* of U :

Definition 2.1. The defect of an $N \times N$ unitary matrix U , denoted $\mathbf{d}(U)$, is the following integer number:

$$\mathbf{d}(U) = (N - 1)^2 - \dim(Df_{\text{vec}_{\mathbb{R}}(U)}(\mathbf{T}_U \mathcal{U})). \tag{4}$$

It is obvious that $\mathbf{d}(U) = d$ is equivalent to the fact that the dimension of the part of the nullspace of $Df_{\text{vec}_{\mathbb{R}}(U)}$ contained in $\mathbf{T}_U \mathcal{U}$ is equal to

$$\begin{aligned} \dim(\text{null}_{\mathbb{R}}(Df_{\text{vec}_{\mathbb{R}}(U)}) \cap \mathbf{T}_U \mathcal{U}) &= \dim(\mathbf{T}_U \mathcal{U}) - \dim(\mathbf{T}_f(\text{vec}_{\mathbb{R}}(U))\mathcal{B}) + d \\ &= N^2 - (N - 1)^2 + d = 2N - 1 + d. \end{aligned} \tag{5}$$

If $\mathbf{d}(U) > 0$ then $\text{vec}_{\mathbb{R}}(U)$ is also called a *critical point* of map f restricted to \mathcal{U} .

2.2. Other characterizations of the defect

The tangent space $\mathbf{T}_U \mathcal{U}$ is equal to the set:

$$\begin{aligned} \{\text{vec}_{\mathbb{R}}(EU) : E \text{ anti-hermitian}\} &= \text{(or alternatively),} \\ \{\text{vec}_{\mathbb{R}}(UF) : F \text{ anti-hermitian}\} \end{aligned} \tag{6}$$

and is spanned by all the independent vectors from the set:

$$\{\text{vec}_{\mathbb{R}}(A^{(i,j)}U) : 1 \leq i < j \leq N\} \cup \{\text{vec}_{\mathbb{R}}(S^{(i,j)}U) : 1 \leq i \leq j \leq N\}, \tag{7}$$

where

$$A_{k,l}^{(i,j)} = \begin{cases} 1 & \text{for } (k, l) = (i, j), \\ -1 & \text{for } (k, l) = (j, i), \\ 0 & \text{otherwise,} \end{cases} \quad S_{k,l}^{(i,j)} = \begin{cases} \mathbf{i} & \text{for } (k, l) = (i, j), \\ \mathbf{i} & \text{for } (k, l) = (j, i), \\ 0 & \text{otherwise,} \end{cases} \tag{8}$$

$$1 \leq i < j \leq N, \quad 1 \leq i \leq j \leq N$$

as matrices $A^{(i,j)}$ and $S^{(i,j)}$ span the real space of anti-hermitian matrices.

Since $Df_{\text{vec}_{\mathbb{R}}(U)}(\text{vec}_{\mathbb{R}}(S^{(i,i)}U)) = \mathbf{0}$ we consider only ordered pairs (i, j) , $i < j$, in construction of a matrix M containing vectors spanning $Df_{\text{vec}_{\mathbb{R}}(U)}(\mathbf{T}_U \mathcal{U})$ as its columns.

First, let us construct an $N^2 \times N(N - 1)/2$ complex matrix $M_{\mathbb{C}}$ such that it's $\alpha(i, j)$ th column (see Appendix A for $\alpha(\cdot, \cdot)$) is defined by

$$[M_{\mathbb{C}}]_{1:N^2, \alpha(i,j)} = \mathbf{vec}_{\mathbb{C}}(U^{(i,j)}), \tag{9}$$

where $U^{(i,j)}$ is an $N \times N$ complex matrix, with the i th and j th non-zero rows only, being negations of each other:

$$\begin{aligned} [U^{(i,j)}]_{i,1:N} &= U_{i,1:N} \circ \overline{U}_{j,1:N}, \\ [U^{(i,j)}]_{j,1:N} &= -U_{i,1:N} \circ \overline{U}_{j,1:N}. \end{aligned} \tag{10}$$

Secondly, we form an $N^2 \times N(N - 1)$ real matrix M ,

$$M = [\mathbf{Re}(M_{\mathbb{C}}) | \mathbf{Im}(M_{\mathbb{C}})], \tag{11}$$

which has that nice property:

$$\begin{aligned} M_{1:N^2, \alpha(i,j)} &= [\mathbf{Re}(M_{\mathbb{C}})]_{1:N^2, \alpha(i,j)} = Df_{\mathbf{vec}_{\mathbb{R}}(U)}(\mathbf{vec}_{\mathbb{R}}(A^{(i,j)}U)), \\ M_{1:N^2, \frac{N(N-1)}{2} + \alpha(i,j)} &= [\mathbf{Im}(M_{\mathbb{C}})]_{1:N^2, \alpha(i,j)} = Df_{\mathbf{vec}_{\mathbb{R}}(U)}(\mathbf{vec}_{\mathbb{R}}(S^{(i,j)}U)). \end{aligned} \tag{12}$$

Hence $\mathbf{span}_{\mathbb{R}}(M) = Df_{\mathbf{vec}_{\mathbb{R}}(U)}(\mathbf{T}_U \mathcal{U})$, and the defect of U can be calculated as

$$\mathbf{d}(U) = (N - 1)^2 - \mathbf{rank}(M). \tag{13}$$

Note also that

$$\dim(\mathbf{null}_{\mathbb{R}}(M^T)) = N^2 - \dim(\mathbf{span}_{\mathbb{R}}(M^T)), \tag{14}$$

where

$$\dim(\mathbf{span}_{\mathbb{R}}(M^T)) = \dim(\mathbf{span}_{\mathbb{R}}(M)) = (N - 1)^2 - \mathbf{d}(U), \tag{15}$$

so

$$\begin{aligned} \mathbf{d}(U) &= N^2 - (2N - 1) - \dim(\mathbf{span}_{\mathbb{R}}(M^T)) \\ &= \dim(\mathbf{null}_{\mathbb{R}}(M^T)) - (2N - 1). \end{aligned} \tag{16}$$

The nullspace of M^T is the solution to the real system

$$M^T \cdot \mathbf{vec}(R) = \mathbf{0} \tag{17}$$

with respect to a real $N \times N$ matrix variable R , which can be rewritten with the matrix $M_{\mathbb{C}}$:

$$M_{\mathbb{C}}^T \cdot \mathbf{vec}(R) = \mathbf{0}, \tag{18}$$

or explicitly

$$\forall 1 \leq i < j \leq N, \quad \sum_{k=1}^N U_{i,k} \overline{U}_{j,k} (R_{i,k} - R_{j,k}) = 0. \tag{19}$$

System (19) is solved by the $(2N - 1)$ dimensional real space spanned by matrices with only one row, or only one column, filled with 1's, the other elements being zeros. If the real solution space of (19) is not greater than that, then $\mathbf{d}(U) = 0$ according to the alternative definition (16) of the defect.

The solution space of system (19) can also be expressed as

$$\begin{aligned} \{R : iR \circ U = EU \text{ for some anti-Hermitian } E\} &= \text{(or alternatively),} \\ \{R : (iR \circ U)U^* \text{ is anti-Hermitian}\}, \end{aligned} \tag{20}$$

that is the set of those R , for which the direction $\text{vec}_{\mathbb{R}}(\mathbf{i}R \circ U)$ of the zero first order change of moduli of matrix U sitting in $\text{vec}_{\mathbb{R}}(U)$ belongs to the tangent space $\mathbf{T}_U \mathcal{U}$.

Those special R 's that solve (19), give rise, through $R \rightarrow \mathbf{i}R \circ U$, to matrices $\mathbf{i} \cdot \text{diag}(e_k) \cdot U, U \cdot \mathbf{i} \cdot \text{diag}(e_k)$, which satisfy the equality in the definition of the set in (20). If a matrix U has no zero entries, like in the case of unitary complex Hadamard matrices, then these matrices span a $(2N - 1)$ dimensional real space, which can be represented in the vector form,

$$\text{span}_{\mathbb{R}}(\{\text{vec}_{\mathbb{R}}(\mathbf{i} \cdot \text{diag}(e_k) \cdot U): k = 1, \dots, N\} \cup \{\text{vec}_{\mathbb{R}}(U \cdot \mathbf{i} \cdot \text{diag}(e_k)): k = 1, \dots, N\}). \tag{21}$$

This is due to the fact that for linear combinations we have this equivalence with the special R 's, $e_k \mathbf{e}^T, \mathbf{e} e_k^T$ (for \mathbf{e} see Appendix A):

$$\begin{aligned} \sum_{k=1}^N \alpha_k \text{vec}_{\mathbb{R}}(\mathbf{i} \cdot \text{diag}(e_k) \cdot U) + \sum_{l=1}^N \beta_l \text{vec}_{\mathbb{R}}(U \cdot \mathbf{i} \cdot \text{diag}(e_l)) &= \mathbf{0}, \\ \Downarrow \\ \sum_{k=1}^N \alpha_k \cdot e_k \mathbf{e}^T + \sum_{l=1}^N \beta_l \cdot \mathbf{e} e_l^T &= \mathbf{0} \end{aligned} \tag{22}$$

if $|U_{i,j}| \neq 0$ for $i, j \in \{1, \dots, N\}$. Also in this case, the vectors

$$\text{vec}_{\mathbb{R}}(\mathbf{i} \cdot \text{diag}(e_k) \cdot U), \quad k = 1, \dots, N \quad \text{and} \quad \text{vec}_{\mathbb{R}}(U \cdot \mathbf{i} \cdot \text{diag}(e_l)), \quad l = 2, \dots, N \tag{23}$$

span the space tangent at $\text{vec}_{\mathbb{R}}(U)$ to a $(2N - 1)$ dimensional manifold:

$$\{\text{vec}_{\mathbb{R}}(\text{diag}(e^{i\alpha_1}, \dots, e^{i\alpha_N}) \cdot U \cdot \text{diag}(1, e^{i\beta_2}, \dots, e^{i\beta_N})) : \alpha_k, \beta_k \in \mathbb{R}\} \tag{24}$$

and if $\mathbf{d}(U) = d > 0$ then these vectors, together with additional independent vectors v_1, \dots, v_d , form a basis for the space

$$\text{null}_{\mathbb{R}}(Df_{\text{vec}_{\mathbb{R}}(U)}) \cap \mathbf{T}_U \mathcal{U}. \tag{25}$$

In general, vectors (23) always belong to the above space, but they may span a space of dimension smaller than $(2N - 1)$ (and not greater, through the \Uparrow implication in (22) for $\alpha_k = -\beta_l = 1$). Then also the manifold (24), obtained from U by the left and the right multiplication of U by unitary diagonal matrices, will have its dimension reduced. This is the subject of Lemma 3.6 in Section 3.

In section 4.2 we are going to apply another characterization of the defect. New formulae and the ones already introduced, all of which will later be used when proving various properties of the defect, are summarized by the following lemma.

Lemma 2.2. *The defect of an $N \times N$ unitary matrix U can be calculated as*

$$\mathbf{d}(U) = \dim(\text{null}_{\mathbb{R}}(M^T)) - (2N - 1) \tag{26}$$

$$= (N - 1)^2 - \dim(\text{span}_{\mathbb{R}}(M)) \tag{27}$$

$$= \dim(\text{null}_{\mathbb{C}}(W^T)) - (2N - 1) \tag{28}$$

$$= (N - 1)^2 - \dim(\text{span}_{\mathbb{C}}(W)), \tag{29}$$

where (with $M_{\mathbb{C}}$ of (9))

$$W = [M_{\mathbb{C}} | -\overline{M_{\mathbb{C}}}] \tag{30}$$

Proof. Only the formulas (28) and (29) need explanation. Note that

$$v \in \text{null}_{\mathbb{C}}(W^T) \implies \bar{v}, \text{Re}(v), \text{Im}(v) \in \text{null}_{\mathbb{C}}(W^T), \tag{31}$$

$$r \text{ real} \in \text{null}_{\mathbb{C}}(W^T) \implies r \in \text{null}_{\mathbb{R}}(M^T), \tag{32}$$

$$r \in \text{null}_{\mathbb{R}}(M^T) \implies r \in \text{null}_{\mathbb{C}}(W^T). \tag{33}$$

Let $R_i, i = 1, \dots, N$, denote matrices with the i th row filled with 1's, having 0's elsewhere, and let $C_j, j = 2, \dots, N$, denote matrices with the j th column filled with 1's, having 0's elsewhere. Obviously, $\text{vec}(R_i), \text{vec}(C_j) \in \text{null}_{\mathbb{R}}(M^T), \text{null}_{\mathbb{C}}(W^T)$, and they are all independent.

Let vectors $v_1, \dots, v_d \in \mathbb{C}^N$ be such that the set of complex vectors

$$\{v_l: l = 1, \dots, d\} \cup \{\text{vec}(R_i): i = 1, \dots, N\} \cup \{\text{vec}(C_j): j = 2, \dots, N\} \tag{34}$$

is contained in $\text{null}_{\mathbb{C}}(W^T)$ and consists of independent vectors. In this reasoning the case when $d = 0$, that is when $\{v_1, \dots, v_d\}$ is empty, is included.

Then one can choose real vectors $r_1, \dots, r_d \in \{\text{Re}(v_l), \text{Im}(v_l): l = 1, \dots, d\}$ such that the set of real vectors

$$\{r_l: l = 1, \dots, d\} \cup \{\text{vec}(R_i): i = 1, \dots, N\} \cup \{\text{vec}(C_j): j = 2, \dots, N\} \tag{35}$$

is contained in $\text{null}_{\mathbb{R}}(M^T)$ and consists of independent vectors.

This choice is possible due to the following inclusion relation:

$$\begin{aligned} &\text{span}_{\mathbb{C}}(\{v_l: l = 1, \dots, d\} \cup \{\text{vec}(R_i): i = 1, \dots, N\} \cup \{\text{vec}(C_j): j = 2, \dots, N\}) \\ &\subset \text{span}_{\mathbb{C}}(\{\text{Re}(v_l), \text{Im}(v_l): l = 1, \dots, d\} \cup \{\text{vec}(R_i): i = 1, \dots, N\} \\ &\cup \{\text{vec}(C_j): j = 2, \dots, N\}). \end{aligned} \tag{36}$$

On the other hand, if we assume that all the vectors in the set (35) are independent and belong to $\text{null}_{\mathbb{R}}(M^T)$, then they form an independent set, as complex vectors, in $\text{null}_{\mathbb{C}}(W^T)$.

Thus we have come to that:

$$\dim(\text{null}_{\mathbb{R}}(M^T)) = \dim(\text{null}_{\mathbb{C}}(W^T)). \quad \square \tag{37}$$

To provide yet another characterization of the defect of U , used later in section 4.1 in the proof of Theorem 4.2, let us define a function $g : \mathbb{R}^{N^2} \longrightarrow \mathbb{R}^{N(N-1)}$ (g will also occur in section 6 in the proof of Theorem 6.3) :

$$\begin{aligned} [g(\text{vec}(R))]_{\alpha(i,j)} &= \text{Re} \left(-\mathbf{i} \cdot \sum_{k=1}^N U_{i,k} \overline{U}_{j,k} e^{\mathbf{i}(R_{i,k} - R_{j,k})} \right), \quad 1 \leq i < j \leq N, \\ [g(\text{vec}(R))]_{\frac{N(N-1)}{2} + \alpha(i,j)} &= \text{Im} \left(-\mathbf{i} \cdot \sum_{k=1}^N U_{i,k} \overline{U}_{j,k} e^{\mathbf{i}(R_{i,k} - R_{j,k})} \right), \quad 1 \leq i < j \leq N. \end{aligned} \tag{38}$$

Note that $g(\text{vec}(R)) = \mathbf{0}$ precisely corresponds to the condition that matrix $U \circ \mathbf{EXP}(\mathbf{i}R)$ is unitary. At this moment recall that $f - f(U)$ can be interpreted as a function characterizing deviations of the moduli of an argument V with respect to the moduli of U while moving V along \mathcal{U} . On the other hand, the function g measures deviation of $U \circ \mathbf{EXP}(\mathbf{i}R)$ from unitarity along the set of matrices with constant moduli.

The value of the linear map $Dg_0 : \mathbb{R}^{N^2} \rightarrow \mathbb{R}^{N(N-1)}$, being the differential of g at $\mathbf{0}$, at $\mathbf{vec}(R)$, is the vector

$$\begin{aligned}
 [Dg_0(\mathbf{vec}(R))]_{\alpha(i,j)} &= \mathbf{Re} \left(\sum_{k=1}^N U_{i,k} \bar{U}_{j,k} (R_{i,k} - R_{j,k}) \right), \quad 1 \leq i < j \leq N, \\
 [Dg_0(\mathbf{vec}(R))]_{\frac{N(N-1)}{2} + \alpha(i,j)} &= \mathbf{Im} \left(\sum_{k=1}^N U_{i,k} \bar{U}_{j,k} (R_{i,k} - R_{j,k}) \right), \quad 1 \leq i < j \leq N.
 \end{aligned}
 \tag{39}$$

The kernel of the differential Dg_0 corresponds to space of solutions of system (19):

$$\mathbf{d}(U) = \dim(\mathbf{null}_{\mathbb{R}}(Dg_0)) - (2N - 1).
 \tag{40}$$

3. Properties of the defect

Lemma 3.1. For any $N \times N$ unitary matrix U and permutation matrices P_r, P_c :

$$\mathbf{d}(P_r \cdot U \cdot P_c) = \mathbf{d}(U).
 \tag{41}$$

Proof. Consider $M_{\mathbb{C}}^U$ of (9) and M^U of (11), constructed for U , and consider also $M_{\mathbb{C}}^{UP}$ and M^{UP} constructed for UP , where P is a permutation matrix. Then, for I being the $N \times N$ identity matrix,

$$M_{\mathbb{C}}^{UP} = (I \otimes P^T) M_{\mathbb{C}}^U \implies M^{UP} = (I \otimes P^T) M^U,
 \tag{42}$$

which, using (13), results in $\mathbf{d}(UP) = \mathbf{d}(U)$.

Now, let P be given by $P_{i,:} = e_{\sigma(i)}^T$, σ being a permutation map. Then $M_{\mathbb{C}}^{PU}$ of (9) for unitary PU is obtained from $M_{\mathbb{C}}^U$ in the following steps:

- negate and conjugate the $\alpha(i, j)$ th column of $M_{\mathbb{C}}^U$ if $\sigma^{-1}(i) > \sigma^{-1}(j)$, for all $1 \leq i < j \leq N$
- if $\sigma^{-1}(i) < \sigma^{-1}(j)$ shift the $\alpha(i, j)$ th column of the result into the $\alpha(\sigma^{-1}(i), \sigma^{-1}(j))$ th position within a new result, otherwise shift it into the $\alpha(\sigma^{-1}(j), \sigma^{-1}(i))$ th position, for all $1 \leq i < j \leq N$
- left multiply the result by $P \otimes I$

which amounts to permuting and negating columns of M^U to get the corresponding M^{PU} . Thus again $\mathbf{d}(PU) = \mathbf{d}(U)$. \square

Lemma 3.2. For any $N \times N$ unitary matrix U and unitary diagonal matrices D_r, D_c :

$$\mathbf{d}(D_r \cdot U \cdot D_c) = \mathbf{d}(U).
 \tag{43}$$

Proof. Right multiplication of U by D_c brings no change to $M_{\mathbb{C}}$. Left multiplication by D_r stiffly rotates the chains of coefficients

$$(U_{i,1} \bar{U}_{j,1}, U_{i,2} \bar{U}_{j,2}, \dots, U_{i,N} \bar{U}_{j,N})
 \tag{44}$$

of system (19), so it does not change the space of its solutions nor the value of the defect (16). (This rotation is equivalent to right multiplication of each $N^2 \times 2$ sub-matrix of M composed of the real and imaginary part of some column of $M_{\mathbb{C}}$, by a 2×2 real orthogonal matrix.) \square

Lemma 3.3. For any $N \times N$ unitary matrix U

$$\mathbf{d}(U) = \mathbf{d}(U^T) = \mathbf{d}(U^*) = \mathbf{d}(\overline{U}). \tag{45}$$

Proof. Since $M_C^{\overline{U}} = \overline{M_C^U}$, for the M_C matrices of (9) constructed for \overline{U} and U , we have that $M^{\overline{U}}$ is obtained from M^U by negating the right $N^2 \times N(N - 1)/2$ sub-matrix of M^U , which leads to $\mathbf{d}(\overline{U}) = \mathbf{d}(U)$ by (13).

As for U^T , we will show that the set (20), used in characterization of the defect, constructed either for U or U^T , is a linear space of a fixed dimension. Let \mathcal{A} denote the set of all $N \times N$ anti-hermitian matrices, R denotes a real matrix. There holds

$$\begin{aligned} & \{R : \mathbf{i}R \circ U^T = EU^T \text{ for some } E \in \mathcal{A}\} \\ & = \{R : \mathbf{i}R^T \circ U = (UE^T U^*)U \text{ for some } (UE^T U^*) \in \mathcal{A}\} \\ & = \{R : \mathbf{i}R \circ U = EU \text{ for some } E \in \mathcal{A}\}^T. \end{aligned} \tag{46}$$

Thus the system (19) (equivalently system (17)) solved either for U or for U^T yields the solution space of the same dimension in both cases. By (16) then $\mathbf{d}(U) = \mathbf{d}(U^T)$.

Let us recall the definition of an equivalence class in the set of unitary matrices [8,15].

Definition 3.4. Two $N \times N$ unitary matrices U and V are \simeq *equivalent* if there exist permutation matrices P_r, P_c and unitary diagonal matrices D_r, D_c such that

$$V = P_r D_r \cdot U \cdot D_c P_c. \tag{47}$$

Lemmas 3.1 and 3.2 imply that for any two \simeq equivalent unitary matrices, $V \simeq U$, their defect is the same, $\mathbf{d}(V) = \mathbf{d}(U)$. In particular, the defect is constant over the set of all unitary matrices obtained from U by left and right multiplying it by unitary diagonal matrices. This set is the image under $\mathbf{vec}_{\mathbb{R}}^{-1}$ of what we shall call the phasing manifold for U :

Definition 3.5. The *phasing manifold* for a unitary $N \times N$ matrix U is the set

$$\{\mathbf{vec}_{\mathbb{R}}(D_r \cdot U \cdot D_c) : D_r, D_c \text{ unitary diagonal}\}. \tag{48}$$

The phasing manifold for U is a differentiable manifold. Its dimension cannot be greater than $2N - 1$, because any element of (48) can be obtained with D_c having $[D_c]_{1,1} = 1$. More formally, we have

Lemma 3.6. Let

$$\mathbf{span}_{\mathbb{R}}(\{\mathbf{vec}_{\mathbb{R}}(\mathbf{i} \cdot \mathbf{diag}(e_k) \cdot U) : k = 1, \dots, N\} \cup \{\mathbf{vec}_{\mathbb{R}}(U \cdot \mathbf{i} \cdot \mathbf{diag}(e_l)) : l = 1, \dots, N\}) \tag{49}$$

be spanned by all the vectors from the set of independent vectors (where $p + r \leq 2N - 1$):

$$\{\mathbf{vec}_{\mathbb{R}}(\mathbf{i} \cdot \mathbf{diag}(e_{i_k}) \cdot U) : k = 1, \dots, p\} \cup \{\mathbf{vec}_{\mathbb{R}}(U \cdot \mathbf{i} \cdot \mathbf{diag}(e_{j_l})) : l = 1, \dots, r\}. \tag{50}$$

Then the set

$$\{\mathbf{vec}_{\mathbb{R}}(D_r \cdot U \cdot D_c) : D_r, D_c \text{ unitary diagonal}\} \tag{51}$$

is equal to a $(p + r)$ dimensional differential manifold, given by the parametrization:

$$\left\{ \text{vec}_{\mathbb{R}} \left(\text{diag} \left(\text{EXP} \left(\mathbf{i} \sum_{k=1}^p \phi_k e_{i_k} \right) \right) \cdot [U] \cdot \text{diag} \left(\text{EXP} \left(\mathbf{i} \sum_{l=1}^r \psi_l e_{j_l} \right) \right) \right) : \phi_k, \psi_l \in \mathbb{R} \right\}. \tag{52}$$

Proof. First we show that sets (51) and (52) are equal, i.e. that each matrix $D_r U D_c$ can be expressed with D_r, D_c satisfying:

$$[D_r]_{i,i} = 1 \quad \text{for } i \notin \{i_1, \dots, i_p\}, \tag{53}$$

$$[D_c]_{j,j} = 1 \quad \text{for } j \notin \{j_1, \dots, j_r\}. \tag{54}$$

Let

$$V = \text{diag}(e^{i\phi_1}, \dots, e^{i\phi_N}) \cdot U \cdot \text{diag}(e^{i\psi_1}, \dots, e^{i\psi_N}), \tag{55}$$

$$V' = \text{diag}(e^{i\phi'_1}, \dots, e^{i\phi'_N}) \cdot U \cdot \text{diag}(e^{i\psi'_1}, \dots, e^{i\psi'_N}),$$

where

$$\begin{aligned} \phi'_i &= \phi_i + \delta_i \quad \text{if } i \in \{i_1, \dots, i_p\}, & \psi'_j &= \psi_j + \epsilon_j \quad \text{if } j \in \{j_1, \dots, j_r\}, \\ \phi'_i &= 0 \quad \text{if } i \notin \{i_1, \dots, i_p\}, & \psi'_j &= 0 \quad \text{if } j \notin \{j_1, \dots, j_r\} \end{aligned} \tag{56}$$

and where δ_i, ϵ_j are uniquely defined by the equation:

$$\begin{aligned} & \sum_{i \in \{i_1, \dots, i_p\}} \delta_i \cdot \mathbf{i} \cdot \text{diag}(e_i) \cdot U + \sum_{j \in \{j_1, \dots, j_r\}} \epsilon_j \cdot U \cdot \mathbf{i} \cdot \text{diag}(e_j) \\ &= \sum_{i \notin \{i_1, \dots, i_p\}} \phi_i \cdot \mathbf{i} \cdot \text{diag}(e_i) \cdot U + \sum_{j \notin \{j_1, \dots, j_r\}} \psi_j \cdot U \cdot \mathbf{i} \cdot \text{diag}(e_j). \end{aligned} \tag{57}$$

Let

$$V(t) = \text{diag}(e^{i(\phi_1+t\delta_1)}, \dots, e^{i(\phi_N+t\delta_N)}) \cdot [U] \cdot \text{diag}(e^{i(\psi_1+t\epsilon_1)}, \dots, e^{i(\psi_N+t\epsilon_N)}), \tag{58}$$

where δ_i, ϵ_j are defined by (57) for $i \in \{i_1, \dots, i_p\}, j \in \{j_1, \dots, j_r\}$, and for the remaining i, j we define $\delta_i = -\phi_i, \epsilon_j = -\psi_j$.

Let also L and R denote the left and right hand side of Eq. (57), respectively. Then

$$\begin{aligned} \frac{\delta}{\delta t} V(t) &= \text{diag}(e^{i(\phi_1+t\delta_1)}, \dots, e^{i(\phi_N+t\delta_N)}) \cdot (L - R) \cdot \text{diag}(e^{i(\psi_1+t\epsilon_1)}, \dots, e^{i(\psi_N+t\epsilon_N)}) \\ &= \mathbf{0}, \end{aligned} \tag{59}$$

so

$$V = V(0) = V(1) = V' \tag{60}$$

from which it generally follows that sets (51) and (52) are equal.

The equality $V = V'$ can be verified entry by entry, using (57), without derivatives. Then one has to consider cases corresponding to possible answers to the question whether i and j from the index pair i, j of an entry belong or not to $\{i_1, \dots, i_p\}, \{j_1, \dots, j_r\}$, respectively.

To show that (52) is a $(p + r)$ dimensional differential manifold, we need to check that the derivatives of the vector function in (52) span a $(p + r)$ dimensional tangent space. These derivatives are

$$\left. \frac{\delta}{\delta\phi_k} \text{vec}_{\mathbb{R}}(\dots) \right|_{\phi_k, \psi_l=0} = \text{vec}_{\mathbb{R}}(\mathbf{i} \cdot \text{diag}(e_{i_k}) \cdot U), \tag{61}$$

$$\left. \frac{\delta}{\delta\psi_l} \text{vec}_{\mathbb{R}}(\dots) \right|_{\phi_k, \psi_l=0} = \text{vec}_{\mathbb{R}}(U \cdot \mathbf{i} \cdot \text{diag}(e_{j_l}))$$

and they form the $p + r$ element set (50) which is assumed to consist of independent vectors. Thus (52) is a $p + r$ dimensional manifold around $\text{vec}_{\mathbb{R}}(U)$.

Since left and right multiplication of U by unitary diagonal matrices does not disturb the linear independence of vectors in (50), and since the tangent space for any other $\text{vec}_{\mathbb{R}}(D_r \cdot U \cdot D_c)$ in (52) is spanned by vectors of the form (61), (52) is globally a $(p + r)$ dimensional manifold. \square

We will also provide a lower bound for the defect of a real orthogonal matrix, as well as a formula for the defect of a direct sum of unitary matrices.

Lemma 3.7. (a) *If Q is a real $N \times N$ orthogonal matrix, then*

$$\mathbf{d}(Q) \geq \frac{(N - 1)(N - 2)}{2}. \tag{62}$$

(b) *If U is an $N \times N$ block diagonal unitary matrix,*

$$U = U_1 \oplus U_2 \oplus \dots \oplus U_r, \tag{63}$$

with U_1 of size N_1, \dots, U_r of size N_r , then

$$\mathbf{d}(U) = \left((N - 1)^2 - \sum_{k=1}^r (N_k - 1)^2 \right) + \sum_{k=1}^r \mathbf{d}(U_k) > \sum_{k=1}^r \mathbf{d}(U_k). \tag{64}$$

where $\mathbf{d}(U_k) = 0$ if $N_k = 1$, according to the definition of the defect.

Proof. (a) The $M_{\mathbb{C}}$ matrix of (9) constructed for Q , $M_{\mathbb{C}}^Q$, is a real matrix. Then the corresponding M matrix of (11) is equal to:

$$M^Q = [M_{\mathbb{C}} \mid \mathbf{0}] \tag{65}$$

and its rank is not greater than $(N - 1)N/2$. Then by (13):

$$\mathbf{d}(Q) \geq (N - 1)^2 - \frac{(N - 1)N}{2} = \frac{(N - 1)(N - 2)}{2}. \tag{66}$$

(b) The $M_{\mathbb{C}}$ matrix for $U = U_1 \oplus \dots \oplus U_r$, $M_{\mathbb{C}}^U$, can be permuted to take the form:

$$M_{\mathbb{C}}^{U_1} \oplus M_{\mathbb{C}}^{U_2} \oplus \dots \oplus M_{\mathbb{C}}^{U_r} \oplus [\mathbf{0}] \tag{67}$$

and consequently M^U can be permuted to become:

$$M^{U_1} \oplus M^{U_2} \oplus \dots \oplus M^{U_r} \oplus [\mathbf{0}], \tag{68}$$

where those summands M^{U_k} for which $N_k = 1$ are ‘empty’ matrices, that is they do not enter the direct sum.

Then by (13):

$$\begin{aligned} \mathbf{d}(U) &= (N - 1)^2 - \text{rank}(M^U) \\ &= (N - 1)^2 - \sum_{k=1}^r (N_k - 1)^2 + \sum_{k=1}^r ((N_k - 1)^2 - \text{rank}(M^{U_k})) \end{aligned}$$

$$= \left((N - 1)^2 - \sum_{k=1}^r (N_k - 1)^2 \right) + \sum_{k=1}^r \mathbf{d}(U_k), \tag{69}$$

where in the second expression we define $\mathbf{rank}(M^{U_k}) = 0$ if M^{U_k} is ‘empty’. As $\mathbf{d}(U_k) = 0$ if $N_k = 1$, the above formula is also valid in the case of presence of 1×1 diagonal blocks in U . \square

4. Exemplary applications

4.1. Isolated unitary matrices and continuous families of unitary matrices with a fixed pattern of the moduli

Definition 4.1. An $N \times N$ unitary matrix is called *isolated* if there is a neighbourhood \mathcal{W} around $\mathbf{vec}_{\mathbb{R}}(U)$ such that all unitaries V with the properties:

- V has the same pattern of moduli as U , i.e. $|V_{i,j}| = |U_{i,j}|$.
- $\mathbf{vec}_{\mathbb{R}}(V) \in \mathcal{W}$.

are those given by the intersection

$$\mathbf{vec}_{\mathbb{R}}^{-1}(\mathcal{W}) \cap \{D_r \cdot U \cdot D_c : D_r, D_c \text{ unitary diagonal}\}. \tag{70}$$

A one way criterion for some U being isolated, associated with calculation of the defect of U , is stated as follows:

Theorem 4.2. *If the defect $\mathbf{d}(U) = 0$, then matrix U is isolated.*

Proof. All the matrices with the same pattern of the moduli as in U are given by

$$U \circ \mathbf{EXP}(\mathbf{i} \cdot R), \quad \mathbf{vec}(R) \in \mathbb{R}^{N^2}, \tag{71}$$

and the unitarity condition for them can be expressed as

$$-\mathbf{i} \cdot \sum_{k=1}^N U_{i,k} \bar{U}_{j,k} e^{\mathbf{i}(R_{i,k} - R_{j,k})} = 0, \quad 1 \leq i < j \leq N. \tag{72}$$

We can rewrite (72) with the use of function g defined in (38) as

$$g(\mathbf{vec}(R)) = \mathbf{0}. \tag{73}$$

From the characterization of the defect of U with the kernel of the differential of g at $\mathbf{0}$, see (40), we have that condition $\mathbf{d}(U) = 0$ implies $\mathbf{rank}(Dg_{\mathbf{0}}) = N^2 - (2N - 1)$. Then one can choose a subsystem of system (73), consisting of $N^2 - (2N - 1)$ equations

$$\tilde{g}(\mathbf{vec}(R)) = \mathbf{0} \tag{74}$$

with the full rank

$$\dim(D\tilde{g}_{\mathbf{0}}(\mathbb{R}^{N^2})) = N^2 - (2N - 1). \tag{75}$$

System (74) thus defines a $(2N - 1)$ dimensional manifold around $\mathbf{0}$.

This must be a $(2N - 1)$ dimensional space:

$$\left\{ \mathbf{vec} \left(\sum_{k=1}^N \alpha_k (e_k \mathbf{e}^T) + \sum_{l=2}^N \beta_l (\mathbf{e} e_l^T) \right) : \alpha_k, \beta_l \in \mathbb{R} \right\}. \tag{76}$$

If $\mathbf{vec}_{\mathbb{R}}(U \circ \mathbf{EXP}(\mathbf{iR}))$ is in \mathcal{W} , a small neighbourhood of $\mathbf{vec}_{\mathbb{R}}(U)$, it can be expressed with $\mathbf{vec}(R)$ in a certain neighbourhood of $\mathbf{0}$. (The latter neighbourhood can be made sufficiently small by decreasing the size of \mathcal{W} , for the purpose of the next argument.)

If $U \circ \mathbf{EXP}(\mathbf{iR})$ is unitary, then $\mathbf{vec}(R)$ in this neighborhood of $\mathbf{0}$ must satisfy system (73), hence system (74), so it must belong to (76). Thus $U \circ \mathbf{EXP}(\mathbf{iR})$ must be of the form:

$$\mathbf{diag}(e^{i\alpha_1}, \dots, e^{i\alpha_N}) \cdot U \cdot \mathbf{diag}(1, e^{i\beta_2}, \dots, e^{i\beta_N}), \tag{77}$$

that is it belongs to the phasing manifold for U (Definition 3.5). \square

In general, the defect of U allows us to calculate an upper bound for the dimension of a differential manifold \mathcal{F}' , stemming from $\mathbf{vec}_{\mathbb{R}}(U)$, generated by unitary matrices with the same pattern of the moduli as in U , if \mathcal{F}' exists:

$$\mathcal{F}' \subset \{ \mathbf{vec}_{\mathbb{R}}(V) : V \in \mathcal{U} \text{ and } (|V_{i,j}| = |U_{i,j}| \text{ for } i, j \in \{1, \dots, N\}) \}. \tag{78}$$

Such manifolds exist, the phasing manifold (Definition 3.5) being a trivial example.

What is even more important for us, we will consider *dephased* manifolds of this kind. By a dephased manifold we mean a manifold \mathcal{F} with the property described in this definition:

Definition 4.3. A manifold (set) \mathcal{F} , consisting of vector forms $\mathbf{vec}_{\mathbb{R}}(V)$ of unitary matrices V with the moduli of their entries fixed at some nonnegative values, is called a *dephased manifold (set)* if the condition holds:

$$(\mathbf{vec}_{\mathbb{R}}(V) \in \mathcal{F} \text{ and } D_r \cdot V \cdot D_c \neq V) \implies \mathbf{vec}_{\mathbb{R}}(D_r \cdot V \cdot D_c) \notin \mathcal{F} \tag{79}$$

for any unitary diagonal matrices D_r, D_c .

The importance of this subclass of manifolds comes from our interest in determining all \simeq -inequivalent (see Definition 3.4) unitary matrices with the same pattern of the moduli, in particular unitary complex Hadamard matrices. This question is connected to the unistochasticity problem of Section 4.3. And the remark below explains this importance more precisely.

Remark 4.4. Let $\mathbf{vec}_{\mathbb{R}}(U)$ belong to such a dephased manifold \mathcal{F} , as described above. The number of different permuted versions of $U: P_r \cdot U \cdot P_c$ is finite, so finite is the number of their images $D_r P_r \cdot U \cdot P_c D_c$ (obtained with the use of unitary diagonal matrices D_r, D_c) whose vector forms sit in \mathcal{F} . This is because there can be at most one image for each $P_r U P_c$ in $\mathbf{vec}_{\mathbb{R}}^{-1}(\mathcal{F})$.

We conclude that there are finitely many vector forms of unitary matrices \simeq -equivalent to U in \mathcal{F} , and that $\mathbf{vec}_{\mathbb{R}}(U)$ has a neighbourhood in \mathcal{F} in which there are no vector forms of matrices \simeq -equivalent to U .

Moreover, there are infinitely many points in this neighbourhood, representing pairwise \simeq -inequivalent unitary matrices, forming a sequence converging to $\mathbf{vec}_{\mathbb{R}}(U)$.

We need the notion of a dephased matrix:

Definition 4.5. Let U be an $N \times N$ unitary matrix such that the linear space

$$\text{span}_{\mathbb{R}}(\{\text{vec}_{\mathbb{R}}(\mathbf{i} \cdot \text{diag}(e_k) \cdot U): k \in \{1, \dots, N\}\} \cup \{\text{vec}_{\mathbb{R}}(U \cdot \mathbf{i} \cdot \text{diag}(e_l)): l \in \{1, \dots, N\}\}) \tag{80}$$

is spanned by $(p + r) \leq 2N - 1$ independent vectors from a spanning set:

$$\mathcal{S} = \{\text{vec}_{\mathbb{R}}(\mathbf{i} \cdot \text{diag}(e_{i_1}) \cdot U), \dots, \text{vec}_{\mathbb{R}}(\mathbf{i} \cdot \text{diag}(e_{i_p}) \cdot U), \text{vec}_{\mathbb{R}}(U \cdot \mathbf{i} \cdot \text{diag}(e_{j_1})), \dots, \text{vec}_{\mathbb{R}}(U \cdot \mathbf{i} \cdot \text{diag}(e_{j_r}))\}. \tag{81}$$

Let \mathcal{S} be a $(p + r)$ element set of index pairs, $\mathcal{S} \subset \{1, \dots, N\} \times \{1, \dots, N\}$, called a *pattern set* onwards, associated with U and the spanning set \mathcal{S} in such a way that

- $(i, j) \in \mathcal{S} \implies U_{i,j} \neq 0$
- $\text{vec}((e_{i_1} \mathbf{e}^T) \circ F), \dots, \text{vec}((e_{i_p} \mathbf{e}^T) \circ F), \text{vec}((\mathbf{e} e_{j_1}^T) \circ F), \dots, \text{vec}((\mathbf{e} e_{j_r}^T) \circ F)$

are independent vectors, where $F = \sum_{(i,j) \in \mathcal{S}} e_i e_j^T$ is a ‘filtering matrix’.

Then an $N \times N$ unitary matrix V , with the same pattern of the moduli as in U , is called *dephased* with respect to U , according to the pattern set \mathcal{S} associated with the spanning set \mathcal{S} , if

$$V_{i,j} = U_{i,j} \quad \text{for any } (i, j) \in \mathcal{S}. \tag{82}$$

We use the notions introduced above in this lemma:

Lemma 4.6. Let V be dephased with respect to U , according to a pattern set \mathcal{S} associated with a spanning set \mathcal{S} .

If $D_r V D_c \neq V$, then $D_r V D_c$ is not dephased (in the same manner), for any unitary diagonal matrices D_r, D_c .

Proof. Using the procedure applied in the proof of Lemma 3.6, one can find D'_r, D'_c such that $D'_r V D'_c = D_r V D_c$, and (where i_k, j_l characterize \mathcal{S} , as in Definition 4.5):

$$\begin{aligned} [D'_r]_{i,i} &= 1 \quad \text{for } i \notin \{i_1, \dots, i_p\}, \\ [D'_c]_{j,j} &= 1 \quad \text{for } j \notin \{j_1, \dots, j_r\}. \end{aligned} \tag{83}$$

If $D'_r V D'_c \neq V$, some of the remaining diagonal entries of $D'_r : [D'_r]_{i_k, i_k} = e^{i\phi_{i_k}}$ and of $D'_c : [D'_c]_{j_l, j_l} = e^{i\psi_{j_l}}$ must differ from 1. Now assume that $D'_r V D'_c$ is also dephased with respect to U , according to the pattern set \mathcal{S} associated with the spanning set \mathcal{S} . Then, for $F = \sum_{(i,j) \in \mathcal{S}} e_i e_j^T$:

$$\begin{aligned} F \circ (D'_r V D'_c) &= F \circ \text{EXP} \left(\mathbf{i} \left(\sum_{k=1}^p \phi_{i_k} e_{i_k} \mathbf{e}^T + \sum_{l=1}^r \psi_{j_l} \mathbf{e} \mathbf{e}_{j_l}^T \right) \right) \circ V \\ &= \text{EXP} \left(\mathbf{i} \left(\sum_{k=1}^p \phi_{i_k} ((e_{i_k} \mathbf{e}^T) \circ F) + \sum_{l=1}^r \psi_{j_l} ((\mathbf{e} e_{j_l}^T) \circ F) \right) \right) \circ (U \circ F) \\ &= U \circ F, \end{aligned} \tag{84}$$

where the last equality is the consequence of the assumption that $D'_r V D'_c$ is also dephased.

Since $U_{i,j} \neq 0$ for $(i, j) \in \mathcal{I}$, the respective phases must be equal to zero:

$$\sum_{k=1}^p \phi_{i_k} ((e_{i_k} \mathbf{e}^T) \circ F) + \sum_{l=1}^r \psi_{j_l} ((\mathbf{e} e_{j_l}^T) \circ F) = \mathbf{0} \tag{85}$$

and, as the vector forms of matrices standing in combination (85) are independent (the property of the pattern set \mathcal{I} , according to which $D'_r V D'_c$ is dephased), all ϕ_{i_k}, ψ_{j_l} are equal to zero, which contradicts that $D'_r V D'_c \neq V$. \square

We will further consider manifolds (stemming from $\mathbf{vec}_{\mathbb{R}}(U)$) of vector forms of matrices V dephased with respect to U in a chosen way. The above lemma implies that such manifolds are dephased in the sense of Definition 4.3.

Theorem 4.7. *Let U be an $N \times N$ unitary matrix and let \mathcal{F} be a differential manifold in \mathbb{R}^{2N^2} stemming from $\mathbf{vec}_{\mathbb{R}}(U)$, generated, through $V \rightarrow \mathbf{vec}_{\mathbb{R}}(V)$, purely by unitary matrices V with the same pattern of the moduli as in U , and dephased with respect to U according to a pattern set \mathcal{I} associated with a spanning set \mathcal{S} .*

Then

$$\dim \mathcal{F} = \dim(\mathbf{T}_U \mathcal{F}) \leq \mathbf{b}(U) \tag{86}$$

where

$\mathbf{T}_U \mathcal{F} \stackrel{\text{def}}{=} \mathbf{T}_{\mathbf{vec}_{\mathbb{R}}(U)} \mathcal{F}$ the space tangent to \mathcal{F} at $\mathbf{vec}_{\mathbb{R}}(U)$,

$\mathbf{b}(U) = \mathbf{d}(U) + (2N - 1) - \sharp_0 U - \sharp \mathcal{S}$, where

$\sharp_0 U$ the number of zero entries in U ,

$\sharp \mathcal{S}$ the number of elements of the spanning set \mathcal{S} , equal to $p + r \leq 2N - 1$, where p, r bear the same meaning as in Definition 4.5.

Proof. Let $v \in \mathbf{T}_U \mathcal{F}$, that is $v = \gamma'(0)$ for some smooth curve $\gamma(t) \subset \mathcal{F}$ such that $\gamma(0) = \mathbf{vec}_{\mathbb{R}}(U)$. Since $\mathbf{vec}_{\mathbb{R}}^{-1}(\gamma) \subset \mathcal{U}$, $v \in \mathbf{T}_U \mathcal{U}$ i.e. it satisfies

$$v = \mathbf{vec}_{\mathbb{R}}(E \cdot U) \quad \text{for some anti-hermitian } E. \tag{87}$$

Since the moduli of the entries of a matrix do not change over $\mathbf{vec}_{\mathbb{R}}^{-1}(\gamma(t))$, $v \in \mathbf{null}_{\mathbb{R}}(Df_{\mathbf{vec}_{\mathbb{R}}(U)})$ of (3), and in particular zero entries stay intact, so v satisfies also:

$$v = \mathbf{vec}_{\mathbb{R}}(\mathbf{i}R \circ U) \quad \text{for some real matrix } R. \tag{88}$$

Thus v belongs to a space parametrized by the solution space of (19) (or equivalently (17)), namely:

$$v \in \mathcal{D} = \{\mathbf{vec}_{\mathbb{R}}(\mathbf{i}R \circ U) : \mathbf{vec}(R) \in \mathcal{R}\}, \tag{89}$$

where

$$\mathcal{R} = \{\mathbf{vec}(R) : \mathbf{i}R \circ U = EU \quad \text{for some anti-hermitian } E\}. \tag{90}$$

Let $\tilde{\mathcal{I}} \subset \{1, \dots, N\} \times \{1, \dots, N\}$ be such that $(i, j) \in \tilde{\mathcal{I}} \Leftrightarrow U_{i,j} = 0$. Because of potential zeros in U , we can reduce the parametrizing space \mathcal{R} of (90):

$$\mathcal{D} = \{\mathbf{vec}_{\mathbb{R}}(\mathbf{i}R \circ U) : \mathbf{vec}(R) \in \mathcal{R}'\}, \tag{91}$$

where

$$\mathcal{R}' = \mathcal{R} \cap \{\mathbf{vec}(R) : \forall (i, j) \in \tilde{\mathcal{I}}, R_{i,j} = 0\}, \tag{92}$$

and since

$$\mathcal{R} = \bigoplus_{(i,j) \in \tilde{\mathcal{I}}} \{\mathbf{vec}(\alpha \cdot e_i e_j^T) : \alpha \in \mathbb{R}\} \oplus \mathcal{R}', \tag{93}$$

we obtain a bound for the dimension of \mathcal{D} of (89) or (91), using the characterization (16) of the defect of U , stated also by Lemma 2.2 :

$$\begin{aligned} \dim(\mathcal{D}) &\leq \dim(\mathcal{R}') = \dim(\mathcal{R}) - \sharp \tilde{\mathcal{I}} \\ &= \mathbf{d}(U) + (2N - 1) - \sharp_0 U, \end{aligned} \tag{94}$$

where also $\mathcal{R} = \mathbf{null}_{\mathbb{R}}(M^T)$ with M of (11).

Further, for ‘filtering matrices’

$$F = \sum_{(i,j) \in \mathcal{I}} e_i e_j^T, \tag{95}$$

$$G = \mathbf{e} \mathbf{e}^T - \sum_{(i,j) \in \tilde{\mathcal{I}}} e_i e_j^T \tag{96}$$

and for all the matrices (see the description of a spanning set in Definition 4.5)

$$\mathbf{i}(e_{i_k} \mathbf{e}^T) \circ U, \quad k = 1, \dots, p, \tag{97}$$

$$\mathbf{i}(\mathbf{e} e_{j_l}^T) \circ U, \quad l = 1, \dots, r, \tag{98}$$

in $\mathbf{vec}_{\mathbb{R}}^{-1}(\mathcal{S})$, vectors

$$\mathbf{vec}_{\mathbb{R}}(\mathbf{i}(e_{i_k} \mathbf{e}^T) \circ G \circ U), \quad k = 1, \dots, p, \tag{99}$$

$$\mathbf{vec}_{\mathbb{R}}(\mathbf{i}(\mathbf{e} e_{j_l}^T) \circ G \circ U), \quad l = 1, \dots, r$$

are still independent.

As the considered manifold \mathcal{F} is composed of $\mathbf{vec}_{\mathbb{R}}(V)$ with V dephased with respect to U , that is with non-zero entries $V_{i,j}$, for $(i, j) \in \mathcal{I}$, fixed, a non-zero $v \in \mathbf{T}_U \mathcal{F}$ must not belong to a $(p + r)$ -dimensional subspace of \mathcal{D} defined with the use of basis vectors (99) by (we parametrize \mathcal{D} with \mathcal{R}' as in (91), hence we use G in the formula below):

$$\mathcal{D}' = \left\{ \mathbf{vec}_{\mathbb{R}} \left(\sum_{k=1}^p \alpha_k \cdot \mathbf{i}(e_{i_k} \mathbf{e}^T) \circ G \circ U + \sum_{l=1}^r \beta_l \cdot \mathbf{i}(\mathbf{e} e_{j_l}^T) \circ G \circ U \right) : \alpha_k, \beta_l \in \mathbb{R} \right\}. \tag{100}$$

If v were in \mathcal{D}' , that is if it were a combination like that in (100), then the dephasing condition would force for this tangent vector that

$$\mathbf{0} = F \circ \mathbf{vec}_{\mathbb{R}}^{-1}(v) = \mathbf{i} \left(\sum_{k=1}^p \alpha_k \cdot (e_{i_k} \mathbf{e}^T) \circ F + \sum_{l=1}^r \beta_l \cdot (\mathbf{e} e_{j_l}^T) \circ F \right) \circ (U \circ F) \tag{101}$$

implying $\alpha_k = 0, \beta_l = 0$, because vector forms of matrices standing in the last combination are independent, being a requirement for the proper choice of a pattern set \mathcal{I} in Definition 4.5.

$\mathbf{T}_U \mathcal{F}$ is thus bound to be contained in some space \mathcal{D}'' such that $\mathcal{D} = \mathcal{D}' \oplus \mathcal{D}''$. The dimension of \mathcal{D}'' reads, using (94):

$$\dim(\mathcal{D}'') = \dim(\mathcal{D}) - \dim(\mathcal{D}') \tag{102}$$

$$= \dim(\mathcal{D}) - (p + r) \tag{103}$$

$$\leq \mathbf{d}(U) + (2N - 1) - \#_0U - \#S,$$

which completes the proof.

Note that if $\mathcal{F}(\dots)$ is a parametrization of \mathcal{F} around $\mathbf{vec}_{\mathbb{R}}(U)$, \mathcal{F} having the properties stated in Theorem 4.7, then

$$\begin{aligned} \mathcal{F}'(\dots) = & \mathbf{vec}_{\mathbb{R}} \left(\mathbf{diag} \left(\mathbf{EXP} \left(\mathbf{i} \sum_{k=1}^p \phi_k \cdot e_{i_k} \right) \right) \right) \\ & \cdot \mathbf{vec}_{\mathbb{R}}^{-1}(\mathcal{F}(\dots)) \cdot \mathbf{diag} \left(\mathbf{EXP} \left(\mathbf{i} \sum_{l=1}^r \psi_l \cdot e_{j_l} \right) \right) \end{aligned} \tag{104}$$

parametrizes a $(p + r) + \dim \mathcal{F}$ dimensional manifold \mathcal{F}' around $\mathbf{vec}_{\mathbb{R}}(U)$. The additional independent vectors (99) spanning (together with a basis of $\mathbf{T}_U \mathcal{F}$) the space $\mathbf{T}_U \mathcal{F}'$ can be obtained by differentiating (104) with respect to ϕ_k, ψ_l . That is to say, $\mathbf{T}_U \mathcal{F}' = \mathcal{D}' \oplus \mathbf{T}_U \mathcal{F}$. \square

Note that the bound $\mathbf{b}(U)$ defined in Theorem 4.7 is independent of the choice of a spanning set for U . Also, it is natural to suppose that for U having a block diagonal structure $U = U_1 \oplus \dots \oplus U_r$ this bound could be the sum of the bounds calculated for its diagonal components. This rule of a total bound, not necessarily our $\mathbf{b}(U)$, being the sum of some bounds for U_p , applies to a very special construction of a manifold \mathcal{F} in Theorem 4.7, in which the direct sum of matrix forms of respective parametrized dephased manifolds constructed for U_1, \dots, U_r is taken to get the matrix form of \mathcal{F} :

$$\mathbf{vec}_{\mathbb{R}}^{-1}(\mathcal{F}) = \mathbf{vec}_{\mathbb{R}}^{-1}(\mathcal{F}_1) \oplus \dots \oplus \mathbf{vec}_{\mathbb{R}}^{-1}(\mathcal{F}_r), \tag{105}$$

and it is because the dimensions of the component manifolds add up to the dimension of \mathcal{F} .

In fact, this rule holds for the quantity $\mathbf{b}(U)$ defined in theorem 4.7.

Lemma 4.8. *Let $U = U_1 \oplus U_2 \oplus \dots \oplus U_r$ be a block diagonal unitary matrix of size N , where N_p denotes the size of U_p . Then*

$$\mathbf{b}(U) = \mathbf{b}(U_1) + \mathbf{b}(U_2) + \dots + \mathbf{b}(U_r) \tag{106}$$

Proof. Let \mathcal{S}_p be a spanning set for U_p . Let us construct a spanning set \mathcal{S} for U using the rules

$$\begin{aligned} \mathbf{vec}_{\mathbb{R}}(\mathbf{i} \cdot \mathbf{diag}(e_k) \cdot U_p) \in \mathcal{S}_p & \implies \mathbf{vec}_{\mathbb{R}} \left(\mathbf{i} \cdot \mathbf{diag} \left(e_{\sum_{m=1}^{p-1} N_m + k} \right) \cdot U \right) \in \mathcal{S}, \\ \mathbf{vec}_{\mathbb{R}}(U_p \cdot \mathbf{i} \cdot \mathbf{diag}(e_l)) \in \mathcal{S}_p & \implies \mathbf{vec}_{\mathbb{R}} \left(U \cdot \mathbf{i} \cdot \mathbf{diag} \left(e_{\sum_{m=1}^{p-1} N_m + l} \right) \right) \in \mathcal{S} \end{aligned} \tag{107}$$

and let every element of \mathcal{S} be put into it in this way. Thus \mathcal{S} is properly constructed and it is clear that every spanning set for U must be created in this manner.

Though it is not a part of the proof, let us mention that a pattern set \mathcal{I} associated with the set \mathcal{S} must have all its elements put into it using the rule:

$$(i, j) \in \mathcal{I}_p \implies \left(\sum_{m=1}^{p-1} N_m + i, \sum_{m=1}^{p-1} N_m + j \right) \in \mathcal{I}, \tag{108}$$

where \mathcal{I}_p 's are some pattern sets associated with the sets \mathcal{S}_p used in the construction of \mathcal{S} .

Therefore,

$$\# \mathcal{S} = \# \mathcal{S}_1 + \# \mathcal{S}_2 + \dots + \# \mathcal{S}_r, \tag{109}$$

where again $\# \mathcal{S}_p$ stands for the number of elements in \mathcal{S}_p .

Using the above equality as well as formula (64) in Lemma 3.7b we find that

$$\begin{aligned} \mathbf{b}(U) &= \mathbf{d}(U) + (2N - 1) - \#_0 U - \# \mathcal{S} \\ &= \left((N - 1)^2 - \sum_{p=1}^r (N_p - 1)^2 \right) + \sum_{p=1}^r \mathbf{d}(U_p) + \left(2 \sum_{p=1}^r N_p - 1 \right) \\ &\quad - \left(N^2 - \sum_{p=1}^r N_p^2 + \sum_{p=1}^r \#_0 U_p \right) - \sum_{p=1}^r \# \mathcal{S}_p \\ &= \sum_{p=1}^r (\mathbf{d}(U_p) + (2N_p - 1) - \#_0 U_p - \# \mathcal{S}_p) \\ &\quad + (N - 1)^2 - \sum_{p=1}^r (N_p - 1)^2 + r - 1 - N^2 + \sum_{p=1}^r N_p^2 = \sum_{p=1}^r \mathbf{b}(U_p). \quad \square \end{aligned} \tag{110}$$

4.2. Relation to results of Nicoara

In a paper [24] on commuting squares of von Neumann algebras Nicoara introduced the ‘span condition’ for such a square to be isolated. Consider the simple case of a commuting square of orthogonal maximal abelian *-subalgebras of the algebra $\mathcal{M}_N(\mathbb{C})$ of complex $N \times N$ matrices:

$$\begin{array}{ccc} \mathcal{D} & \subset & \mathcal{M}_N(\mathbb{C}) \\ \cup & & \cup \\ \mathbb{C} \cdot I & \subset & U^* \mathcal{D} U, \end{array} \tag{111}$$

where $\mathbb{C} \cdot I$ is the algebra of all $N \times N$ scalar matrices, \mathcal{D} the algebra of all $N \times N$ diagonal matrices, U a unitary complex Hadamard matrix, i.e. $|U_{i,j}|^2 = 1/N$. Any abelian *-subalgebra, as closed with respect to the hermitian transposition $(\cdot \cdot)^*$, is unitarily diagonalizable, and if it is maximal, then it is diagonalizable into \mathcal{D} . The property that a commuting square (111) is isolated is equivalent to U being isolated in accordance with Definition 4.1. The span condition in this case reads:

Lemma 4.9. *A unitary complex Hadamard matrix U is isolated if*

$$\dim([\mathcal{D}, U^* \mathcal{D} U]) = (N - 1)^2, \tag{112}$$

where

$$[\mathcal{D}, U^* \mathcal{D} U] \stackrel{\text{def}}{=} \text{span}_{\mathbb{C}}(\{\text{vec}_{\mathbb{C}}(D_1 \cdot U^* D_2 U - U^* D_2 U \cdot D_1) : D_1, D_2 \in \mathcal{D}\}). \tag{113}$$

Condition (112) is equivalent to

$$\dim(\text{span}_{\mathbb{C}}(\{\text{vec}_{\mathbb{C}}(B^{(i,j)}) : i, j \in \{1, \dots, N\}\})) = (N - 1)^2, \tag{114}$$

where $B^{(i,j)}$ is an $N \times N$ matrix filled all with 0's except for the i th row and the i th column:

$$\begin{aligned} B_{i,1:N}^{(i,j)} &= [(U_{j,1}\overline{U}_{j,i}), \dots, (U_{j,i-1}\overline{U}_{j,i}), 0, (U_{j,i+1}\overline{U}_{j,i}), \dots, (U_{j,N}\overline{U}_{j,i})], \\ B_{1:N,i}^{(i,j)} &= -(B_{i,1:N}^{(i,j)})^*, \end{aligned} \tag{115}$$

as for $D_1 = \mathbf{diag}(\alpha_1, \dots, \alpha_N)$, $D_2 = \mathbf{diag}(\beta_1, \dots, \beta_N)$,

$$D_1 \cdot U^* D_2 U - U^* D_2 U \cdot D_1 = \sum_{i,j \in \{1, \dots, N\}} \alpha_i \beta_j \cdot B^{(i,j)}. \tag{116}$$

We will show that the sufficient condition (112) is equivalent to our condition $\mathbf{d}(U) = 0$ for U being isolated. That is, using also Lemma 3.3, that the equivalence holds:

$$\mathbf{d}(U) = 0 \iff \mathbf{d}(U^*) = 0 \iff (114). \tag{117}$$

To show this, take U^* and form matrix W of Lemma 2.2 for U^* :

$$W^{U^*} = \left[M_{\mathbb{C}}^{U^*} \mid -\overline{M}_{\mathbb{C}}^{U^*} \right] \tag{118}$$

then concatenate it horizontally with an $N^2 \times N$ matrix filled only with 0's, and reorder the columns of the resulting matrix to obtain a square matrix B having the property that its k th $N^2 \times N$ sub-matrix, $k = 1, \dots, N$, is equal to

$$\begin{aligned} B_{1:N^2, (k-1)N+1:kN} & \\ &= [\mathbf{vec}_{\mathbb{C}}(U^{*(k,1)}) \mid \dots \mid \mathbf{vec}_{\mathbb{C}}(U^{*(k,k-1)}) \mid \mathbf{0} \mid \mathbf{vec}_{\mathbb{C}}(U^{*(k,k+1)}) \mid \dots \mid \mathbf{vec}_{\mathbb{C}}(U^{*(k,N)})], \end{aligned} \tag{119}$$

where $U^{(i,j)}$ is defined by (10) for $i < j$, and we additionally define:

$$U^{(j,i)} = -\overline{U^{(i,j)}} \quad \text{for } j > i. \tag{120}$$

Then the rows of B correspond to matrices $B^{(i,j)}$:

$$B^{(i,j)} = \mathbf{vec}_{\mathbb{C}}^{-1}((B_{(i-1)N+j, 1:N^2})^T) \tag{121}$$

and thus, also by Lemma 2.2:

$$\begin{aligned} \dim(\mathbf{span}_{\mathbb{C}}(\{\mathbf{vec}_{\mathbb{C}}(B^{(i,j)}) : i, j \in \{1, \dots, N\}\})) & \\ &= \dim(\mathbf{span}_{\mathbb{C}}(B^T)) = \dim(\mathbf{span}_{\mathbb{C}}(B)) \\ &= \dim(\mathbf{span}_{\mathbb{C}}(W^{U^*})) = (N-1)^2 - \mathbf{d}(U^*) = (N-1)^2 - \mathbf{d}(U). \end{aligned} \tag{122}$$

From the above (117) immediately follows. We can formulate yet another characterization of the defect:

$$\mathbf{d}(U) = (N-1)^2 - \dim(\mathbf{span}_{\mathbb{C}}(\{\mathbf{vec}_{\mathbb{C}}(B^{(i,j)}) : i, j \in \{1, \dots, N\}\})) \tag{123}$$

with $B^{(i,j)}$ described by (115).

4.3. The unistochasticity problem

Related to some applications in physics is the unistochasticity problem, that is the problem of extracting full information about a unitary matrix from the moduli of its entries only.

Definition 4.10. An $N \times N$ bistochastic matrix B is called *unistochastic (orthostochastic)* if there exists an $N \times N$ unitary (real orthogonal) matrix U such that $\forall i, j \in \{1, \dots, N\} B_{i,j} = |U_{i,j}|^2$.

In other words, B is unistochastic if $\mathbf{vec}(B) = f(\mathbf{vec}_{\mathbb{R}}(U))$ for some unitary U , having f defined by (2). In physical applications, i, j th entries of B correspond to probabilities of obtaining the i th possible result of an experiment, being one of some chosen N ‘orthogonal’ states of a measured quantum system, given the j th initial state was prepared. In this framework U , a unitary preimage of B , describes possible evolution of the state of the measured system between the moments of preparation and measurement of the state.

A more detailed question concerning the unistochasticity issue is the following: does there exist a unistochastic ball around the flat matrix J_N , $[J_N]_{i,j} = 1/N$, within the Birkhoff’s polytope, the set of all bistochastic matrices? Note that J_N is unistochastic for every N , since the Fourier matrix F_N of (128) is its unitary preimage. A partial answer to the posed question, which uses the notion of the defect, is provided by the lemma:

Theorem 4.11. *Let U be a unitary complex Hadamard matrix, i.e. $|U_{i,j}| = 1/\sqrt{N}$, thus being a unitary preimage of the flat bistochastic matrix, $\mathbf{vec}_{\mathbb{R}}(U) \in f^{-1}(\mathbf{vec}(J_N))$, where $[J_N]_{i,j} = 1/N$.*

If $\mathbf{d}(U) = 0$ then there exists a unistochastic ball around J_N in the set of all bistochastic matrices.

Proof. Consider the maps (differential symbols also denote their matrix representation $[Dp_v]_{i,j} = \frac{\delta p_i}{\delta x_j}(v)$):

- $u : \mathcal{W} \subset \mathbb{R}^{N^2} \longrightarrow \mathbb{R}^{2N^2}$ parametrizing the unitary manifold $\mathbf{vec}_{\mathbb{R}}(\mathcal{U})$ around $\mathbf{vec}_{\mathbb{R}}(U)$, \mathcal{W} open, such that $u(\mathbf{0} \in \mathcal{W}) = \mathbf{vec}_{\mathbb{R}}(U)$. Then $Du_{\mathbf{0}}(\mathbb{R}^{N^2}) = \mathbf{T}_U \mathcal{U}$ and columns of $Du_{\mathbf{0}}$ form a basis of $\mathbf{T}_U \mathcal{U}$.
- $f : \mathbb{R}^{2N^2} \longrightarrow \mathbb{R}^{N^2}$ defined earlier in (2), $[\mathbf{vec}^{-1}(f(\mathbf{vec}_{\mathbb{R}}(U)))]_{i,j} = |U_{i,j}|^2$, a map squaring the moduli of the entries of a complex matrix.
- $m : \mathbb{R}^{N^2} \longrightarrow \mathbb{R}^{(N-1)^2}$, $m(\mathbf{vec}(B)) = \mathbf{vec}(B_{1:N-1,1:N-1})$, where the second \mathbf{vec} is over $(N-1) \times (N-1)$ matrices. m provides a one to one map between bistochastic $N \times N$ matrices and $(N-1) \times (N-1)$ matrices with non-negative entries, $m(\mathbf{vec}(J_N)) = \mathbf{vec}\left(\frac{N-1}{N} J_{N-1}\right)$, $Dm_{\mathbf{vec}(J_N)}(\mathbf{T}_{\mathbf{vec}(J_N)} \mathcal{B}) = \mathbb{R}^{(N-1)^2}$.

Since $\mathbf{d}(U) = 0$, from the definition of the defect $Df_{\mathbf{vec}_{\mathbb{R}}(U)}(\mathbf{T}_U \mathcal{U}) = \mathbf{T}_{\mathbf{vec}(J_N)} \mathcal{B}$, that is an $N^2 \times N^2$ matrix $Df_{\mathbf{vec}_{\mathbb{R}}(U)} \cdot Du_{\mathbf{0}}$ contains a basis for $\mathbf{T}_{\mathbf{vec}(J_N)} \mathcal{B}$, say at $j_1, j_2, \dots, j_{(N-1)^2}$ th column positions.

Consider the map $\tilde{u} : \mathbb{R}^{(N-1)^2} \longrightarrow \mathbb{R}^{2N^2}$, being map u restricted to its j_1 th, \dots , $j_{(N-1)^2}$ th variables, the other variables being set to 0. Then of course columns of $Df_{\mathbf{vec}_{\mathbb{R}}(U)} \cdot D\tilde{u}_{\mathbf{0}}$ form the above basis of $\mathbf{T}_{\mathbf{vec}(J_N)} \mathcal{B}$, and columns of the $(N-1) \times (N-1)$ matrix $Dm_{\mathbf{vec}(J_N)} \cdot Df_{\mathbf{vec}_{\mathbb{R}}(U)} \cdot D\tilde{u}_{\mathbf{0}}$ must form a basis for $\mathbb{R}^{(N-1)^2}$, i.e. this matrix is non-singular.

Thus the differentiable map $m(f(\tilde{u})) : \mathbb{R}^{(N-1)^2} \longrightarrow \mathbb{R}^{(N-1)^2}$ satisfies the Inverse Function Theorem. This means that each point v in an open set $\mathcal{V} \subset \mathbb{R}^{(N-1)^2}$ around $\mathbf{vec}\left(\frac{N-1}{N} J_{N-1}\right)$ has its preimage \tilde{w} in an open set $\tilde{\mathcal{W}} \subset \mathbb{R}^{(N-1)^2}$ containing $\mathbf{0}$.

Consider a ‘pseudo-inverse’ of m : n , such that

$$n(v \in \mathbb{R}^{(N-1)^2}) = \mathbf{vec} \left(\begin{bmatrix} \mathbf{vec}^{-1}(v) & \vdots \\ \dots & \cdot \end{bmatrix} \in \mathcal{B} \right), \tag{124}$$

where the second \mathbf{vec} is over $(N - 1) \times (N - 1)$ matrices, and the N th row and N th column of the matrix in brackets on the right hand side is completed to form a bistochastic matrix. Note that $n(m) = \mathbf{id}$ over $\mathbf{vec}(\mathcal{B})$, and of course $m(n) = \mathbf{id}$.

The stated above property of $m(f(\tilde{u}))$ can now be rephrased as:

Any point $n(v)$ in the set $n(\mathcal{V})$ open in $\mathbf{vec}(\mathcal{B})$ around $\mathbf{vec}(J_N)$, corresponding to a bistochastic matrix $\mathbf{vec}^{-1}(n(v))$, has its preimage $\tilde{u}(\tilde{w}) \in \tilde{\mathcal{U}}(\tilde{\mathcal{W}}) \subset \mathbf{vec}_{\mathbb{R}}(\mathcal{U})$, corresponding to a unitary matrix $\mathbf{vec}_{\mathbb{R}}^{-1}(\tilde{u}(\tilde{w}))$:

$$\begin{aligned} v &= m(f(\tilde{u}(\tilde{w}))) \\ \Downarrow \\ n(v) &= f(\tilde{u}(\tilde{w})). \quad \square \end{aligned} \tag{125}$$

In section 5 we show that the defect of the Fourier matrix F_N is equal to zero only for N prime. Therefore it is tempting to suppose that a unistochastic ball around J_N may not exist for composite N . This is indeed true for $N = 4$, as there exists a ray, stemming from J_4 , of bistochastic matrices with the property that they have not unitary preimages [4]:

$$\left\{ J_4 + t \cdot \begin{bmatrix} \frac{9}{4} & -\frac{3}{4} & -\frac{3}{4} & -\frac{3}{4} \\ -\frac{3}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ -\frac{3}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \\ -\frac{3}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{bmatrix} : t \in \left(-\frac{1}{9}, 0 \right) \right\}. \tag{126}$$

However, for $N = 6$ there exists a unistochastic ball around J_6 . This is because the so called ‘spectral matrix’ S_6 :

$$S_6 = \frac{1}{\sqrt{6}} \cdot \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & \omega & \omega & \omega^2 & \omega^2 \\ 1 & \omega & 1 & \omega^2 & \omega^2 & \omega \\ 1 & \omega & \omega^2 & 1 & \omega & \omega^2 \\ 1 & \omega^2 & \omega^2 & \omega & 1 & \omega \\ 1 & \omega^2 & \omega & \omega^2 & \omega & 1 \end{bmatrix}, \quad \text{where } \omega = \exp\left(\mathbf{i} \cdot \frac{2\pi}{3}\right) \tag{127}$$

found independently by Tao [31] and by Moorhouse [30] (denoted by $S_6^{(0)}$ in our catalogue [15]), has the defect equal to zero, so Theorem 4.11 can be applied. Similar examples for $N = 9$ and $N = 10$ can be found in [27], see matrices H_9 and BN_{10} there (in [15] they are denoted by $N_9^{(0)}$ and $N_{10}^{(0)}$). Thus we also have unistochastic balls around J_9 and J_{10} .

5. The defect of a Fourier matrix

In this section we will use system (19) to obtain the value of defect of the $N \times N$ unitary Fourier matrix F_N ,

$$[F_N]_{i,j} = \frac{1}{\sqrt{N}} e^{\mathbf{i} \frac{2\pi}{N} (i-1)(j-1)}, \quad i, j \in \{1, 2, \dots, N\}. \tag{128}$$

This value, as well as the defect of any unitary complex Hadamard matrix H ($|H_{i,j}| = 1/\sqrt{N}$), is interesting from the point of view of the unistochasticity issue, discussed in the previous subsection. If the defect of such a matrix equals zero then there exists a unistochastic ball around the flat matrix J_N ($[J_N]_{i,j} = 1/N$) in the set of all bistochastic matrices, see Theorem 4.11.

Furthermore, the result $d(F_N) = 0$ implies that the Fourier matrix is isolated, see Theorem 4.2. On the other hand, any positive defect d of a given unitary complex Hadamard matrix H (of which F_N is an example) gives the upper bound for the dimension of a smooth orbit of complex Hadamard matrices, dephased with respect to H , stemming from H . This is stated by Theorem 4.7.

A similar approach, to the one presented below in calculation of the defect, can be used to calculate the defect of any Kronecker product of unitary Fourier matrices. In fact, one needs to calculate the defect only for representatives of permutation equivalence classes of such products, see [26]. For instance, F_6 is permutation equivalent to $F_2 \otimes F_3$, so Lemma 3.1 implies that their defects are equal. On the other hand, $F_4 \otimes F_2 \otimes F_2$ and $F_4 \otimes F_4$ are permutation inequivalent, even if we pre-multiply both products by unitary diagonal matrices [26]. Thus Lemmas 3.1 and 3.2 cannot be used and these defects need not to be equal.

5.1. Statement of the main result

Before we prove a formula for the defect of the Fourier matrix of size N , we need the definition of a *parameter cycle matrix*, in which the notion of least common multiple (**lcm**) is used.

Definition 5.1. A *parameter cycle matrix (PCM)* of size N is any complex $N \times N$ matrix P built using these rules (where $P^{x,y}$ designates parameters in matrix P in a way different from ordinary indexing of rows and columns; we call x the step index and y the cycle index):

- The first column of P is filled with N arbitrary *real* numbers, $P^{0,0}, \dots, P^{0,N-1}$, running from the top to the bottom.
- For the step index $j \in \{2, \dots, \frac{N+1}{2}\}$ if N is odd, or for $j \in \{2, \dots, \frac{N}{2}\}$ if N is even, the j th and $(N - j + 2)$ th column of P are filled in such a way that

$$\begin{aligned}
 P^{j-1,k-1} &= P_{k,j} = P_{(k+(j-1))\bmod N, j} = \dots = P_{\left(k+\left(\frac{\text{lcm}(N,j-1)}{j-1}-1\right)(j-1)\right)\bmod N, j}, \\
 \overline{P^{j-1,k-1}} &= P_{k, N-j+2} = P_{(k+(j-1))\bmod N, N-j+2} \\
 &= \dots = P_{\left(k+\left(\frac{\text{lcm}(N,j-1)}{j-1}-1\right)(j-1)\right)\bmod N, N-j+2},
 \end{aligned}
 \tag{129}$$

where

$$k = 1, 2, \dots, \frac{N}{\frac{\text{lcm}(N,j-1)}{j-1}}
 \tag{130}$$

designates the $(k - 1)$ th $(\text{lcm}(N, j - 1))/(j - 1)$ element ‘cycle’, and $P^{j-1,k-1}$ are arbitrary *complex* parameters of P .

- If N is even, then the $(N/2 + 1)$ th column is filled according to the pattern:

$$P^{\frac{N}{2},k-1} = P_{k, \frac{N}{2}+1} = P_{k+\frac{N}{2}, \frac{N}{2}+1} \quad \text{for } k = 1, 2, \dots, \frac{N}{2},
 \tag{131}$$

where $P^{\frac{N}{2},k-1}$ are arbitrary *real* parameters.

As an example we provide a parameter cycle matrix of order 6,

$$\begin{bmatrix} P^{0,0} & P^{1,0} & P^{2,0} & P^{3,0} & \overline{P^{2,0}} & \overline{P^{1,0}} \\ P^{0,1} & P^{1,0} & P^{2,1} & P^{3,1} & \overline{P^{2,1}} & \overline{P^{1,0}} \\ P^{0,2} & P^{1,0} & P^{2,0} & P^{3,2} & \overline{P^{2,0}} & \overline{P^{1,0}} \\ P^{0,3} & P^{1,0} & P^{2,1} & P^{3,0} & \overline{P^{2,1}} & \overline{P^{1,0}} \\ P^{0,4} & P^{1,0} & P^{2,0} & P^{3,1} & \overline{P^{2,0}} & \overline{P^{1,0}} \\ P^{0,5} & P^{1,0} & P^{2,1} & P^{3,2} & \overline{P^{2,1}} & \overline{P^{1,0}} \end{bmatrix}. \tag{132}$$

The notion of a parameter cycle matrix allows us to obtain concrete results on the defect of the Fourier matrix F_N of size N . It can be expressed with a sum of greatest common divisors (gcd).

Theorem 5.2. For $N \geq 2$ being a natural number

$$d(F_N) = \begin{cases} 1 - N + 2 \sum_{l=1}^{\frac{N-1}{2}} \gcd(N, l) & \text{for } N \text{ odd,} \\ 1 - \frac{N}{2} + 2 \sum_{l=1}^{\frac{N}{2}-1} \gcd(N, l) & \text{for } N \text{ even.} \end{cases}$$

Proof. We rewrite system (19) for F_N , denoted further as F :

$$\forall 1 \leq i < j \leq N, \quad \sum_{k=1}^N F_{i,k} \overline{F_{j,k}} (R_{i,k} - R_{j,k}) = 0 \tag{133}$$

as

$$\sum_{k=1}^N R_{i,k} F_{j-i+1,k} = \sum_{k=1}^N R_{j,k} F_{j-i+1,k} \tag{134}$$

and there also generally holds that

$$\sum_{k=1}^N R_{i,k} F_{j-i+1,k} = \sum_{k=1}^N R_{i,k} \overline{F_{N-(j-i)+1,k}} = \overline{\sum_{k=1}^N R_{i,k} F_{N-(j-i)+1,k}}. \tag{135}$$

We introduce a complex $N \times N$ matrix P such that:

$$\overline{P} \stackrel{\text{def}}{=} R \cdot F^T = R \cdot F \iff P = RF^* \iff R = PF \tag{136}$$

Then statements (134) and (135) can be expressed in terms of the elements of matrix P as

$$\begin{aligned} \overline{P}_{i,j-i+1} &= P_{i,N-(j-i)+1} \\ \parallel & \parallel \\ \overline{P}_{j,j-i+1} &= P_{j,N-(j-i)+1} \end{aligned} \tag{137}$$

Rules (137) as well as the requirement of matrix R being real force matrix P to be a parameter cycle matrix of Definition 5.1, and the solution space of (133) is fully parametrized by the formula $R = PF$, where P is any such PCM matrix.

The total number of *real* parameters in P , parametrizing the solution space of (133), reduced by $(2N - 1)$ to become the defect of F_N , reads

• N odd

$$\begin{aligned} \mathbf{d}(F_N) &= N + 2 \left(\sum_{l=1}^{\frac{N-1}{2}} \frac{N}{\text{lcm}(N,l)} \right) - (2N - 1) \\ &= 2 \sum_{l=1}^{\frac{N-1}{2}} \left(\frac{N}{\text{lcm}(N,l)} - 1 \right) = 2 \sum_{l=1}^{\frac{N-1}{2}} (\text{gcd}(N, l) - 1), \end{aligned}$$

• N even

$$\begin{aligned} \mathbf{d}(F_N) &= N + 2 \left(\sum_{l=1}^{\frac{N}{2}-1} \frac{N}{\text{lcm}(N,l)} \right) + \frac{N}{2} - (2N - 1) \\ &= 2 \sum_{l=1}^{\frac{N}{2}-1} \left(\frac{N}{\text{lcm}(N,l)} - \frac{1}{2} \right) = 2 \sum_{l=1}^{\frac{N}{2}-1} \left(\text{gcd}(N, l) - \frac{1}{2} \right). \end{aligned}$$

That is

$$N \text{ odd: } \mathbf{d}(F_N) = 1 - N + 2 \sum_{l=1}^{\frac{N-1}{2}} \text{gcd}(N, l) \tag{138}$$

$$N \text{ even: } \mathbf{d}(F_N) = 1 - \frac{N}{2} + 2 \sum_{l=1}^{\frac{N}{2}-1} \text{gcd}(N, l) \quad \square \tag{139}$$

Alternative formulas, for the defect of F_N can be useful.

Theorem 5.3. For any natural $N \geq 2$ with the factorization into prime numbers:

$$N = \prod_{j=1}^n p_j^{k_j} \quad p_1 > p_2 > \dots > p_n \tag{140}$$

there holds

$$(a) \mathbf{d}(F_N) = \sum_{l=1}^{N-1} (\text{gcd}(N, l) - 1), \tag{141}$$

$$(b) \mathbf{d}(F_N) = N \cdot \left(\prod_{j=1}^n \left(1 + k_j - \frac{k_j}{p_j} \right) - 2 \right) + 1. \tag{142}$$

The proof is provided in Appendix B.

5.2. Some special cases

Since the explicit formula (142) is not very transparent the defects of Fourier matrices for small dimensions are collected in Table 1.

Table 1
Defect for the Fourier matrix F_N of size N

N	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
$\mathbf{d}(F_N)$	0	0	0	1	0	4	0	5	4	8	0	17	0	12	16	17
N	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32
$\mathbf{d}(F_N)$	0	28	0	33	24	20	0	53	16	24	28	49	0	76	0	49

Let us now discuss some special cases of the formula for the defect of the Fourier matrix F_N .

(i) N is prime.

If $N = p$ then $n = 1, k_1 = 1$, so the right hand side of equation (142) reads $p(2 - 1/p - 2) + 1$ and provides the result $\mathbf{d}(F_p) = 0$ as advertised. Hence the Fourier matrix of a prime dimension is isolated.

(ii) N is a product of two distinct primes.

If $N = pq$ then $n = 2, k_1 = k_2 = 1$ so (142) reads $pq[(2 - 1/p)(2 - 1/q) - 2] + 1$, which gives

$$\mathbf{d}(F_{pq}) = 2(p - 1)(q - 1). \tag{143}$$

It is worth to emphasize that the upper bound $\mathbf{b}(F_{pq})$ (see Eq. (86)) for the dimension of an orbit of dephased unitary complex Hadamard matrices stemming from F_{pq} implied by this formula is exactly twice the dimension D of the orbits actually constructed in [8,12,15] for a product of primes, $D = (p - 1)(q - 1)$. The problem of describing the entire (possibly existing) manifold of dephased unitary complex Hadamard matrices stemming from the Fourier matrix F_{pq} is open even in the simplest case $N = 2 \cdot 3 = 6$ [15], but a recent discovery of a new ‘non-affine’ (according to the proper definition in our catalogue [15]) $N = 6$ orbit of unitary complex Hadamard matrices [27], and some further results seem to suggest that in this case a full 4 dimensional orbit does exist [29].

(iii) N is a product of three distinct primes.

If $N = pqr$ then $n = 3, k_1 = k_2 = k_3 = 1$ and eq. (142) amounts to

$$\mathbf{d}(F_{pqr}) = 2[3pqr - 2(pq + pr + qr) + (p + q + r)]. \tag{144}$$

(iv) N is a power of two. If $N = 2^k$ then $p = 2, n = 1$ and $k_1 = k$, so (142) leads to

$$\mathbf{d}(F_{2^k}) = 2^{k-1}(k - 2) + 1. \tag{145}$$

(v) N is a power of a prime.

If $N = p^k$ then $n = 1$ and $k_1 = k$, so (142) takes the form of:

$$\mathbf{d}(F_{p^k}) = p^{k-1}[(p - 1)k - p] + 1. \tag{146}$$

Interestingly, in this very case the defect is equal to the dimension of the known smooth orbits of dephased unitary complex Hadamard matrices stemming from F_{p^k} , featured in Section 6. This shows that these solutions are complete in the sense that they are not contained in smooth orbits (of the respective type) of a higher dimension.

6. Orbits of the maximal dimension stemming from Fourier matrices of a prime power size

In this section we present examples of $N \times N$ unitary matrices U with no zero entries, for which there exist $\mathbf{d}(U)$ -dimensional smooth families (manifolds) generated, through $V \rightarrow \mathbf{vec}_{\mathbb{R}}(V)$, by unitary matrices V with the same pattern of moduli as in U , and dephased with respect to U .

As U has no zero entries, a spanning set \mathcal{S} for U (see Definition 4.5) will always have $p + r = 2N - 1$ independent vectors as its elements. So, according to Theorem 4.7, a manifold of the type described above will have its dimension bounded just by $\mathbf{d}(U)$.

We will consider Fourier matrices F_{p^k} , of the size being the k th natural power of a prime number p , as examples for which this bound is saturated. To make the notion of being dephased with respect to F_{p^k} precise, as Definition 4.5 requires, and also for practical reasons, we arbitrarily choose the spanning set for F_{p^k} to be

$$\begin{aligned} \mathcal{S}_{F_{p^k}} = & \{ \mathbf{vec}_{\mathbb{R}}(\mathbf{i} \cdot \mathbf{diag}(e_r) \cdot F_{p^k}) : r \in \{1, \dots, p^k\} \} \\ & \cup \{ \mathbf{vec}_{\mathbb{R}}(F_{p^k} \cdot \mathbf{i} \cdot \mathbf{diag}(e_c)) : c \in \{2, \dots, p^k\} \}, \end{aligned} \tag{147}$$

and the pattern set to be

$$\mathcal{I}_{F_{p^k}} = \{(1, 1), (2, 1), \dots, (p^k, 1)\} \cup \{(1, 2), (1, 3), \dots, (1, p^k)\}. \tag{148}$$

In other words, V is dephased with respect to F_{p^k} , according to $\mathcal{I}_{F_{p^k}}$ associated with $\mathcal{S}_{F_{p^k}}$, if the entries in the first row and column of V are equal to the corresponding entries in F_{p^k} , i.e. they are all equal to $1/\sqrt{p^k}$. Of course V is assumed to be a unitary complex Hadamard matrix, that is $VV^* = I$, $|V_{i,j}| = 1/\sqrt{p^k}$ for $i, j = 1, \dots, p^k$.

To construct a $\mathbf{d}(F_{p^k})$ -dimensional manifold, generated by dephased unitary complex Hadamard matrices, stemming from $\mathbf{vec}_{\mathbb{R}}(F_{p^k})$, we have to take a subspace of the space of all parameter cycle matrices (PCM matrices) P of size p^k , introduced in Definition 5.1. Because of the dephasing condition we have to impose on P additional constraints. We have to set all p^k real parameters of P sitting in the first row to zero, and each of the remaining $(p^k - 1)$ (out of the total of $2p^k - 1$ to be fixed) real parameters sitting in the first column to minus the sum of the remaining complex parameters sitting in the same row as the parameter (in the 1-st column) being set. This leaves $\mathbf{d}(F_{p^k})$ real parameters free. Then the second column of P as well as each j th column with $(j - 1)$ not divided by p are filled all with zeros. Using these constraints as well as the alternative indexing of parameters in P (see Definition 5.1), we state that:

Theorem 6.1. *The $\mathbf{d}(F_{p^k})$ -parameter family*

$$\left\{ \mathbf{vec}_{\mathbb{R}}(F_{p^k} \circ \mathbf{EXP}(\mathbf{i}PF_{p^k})) : P \text{ is PCM, and } \begin{pmatrix} P^{j,0} = 0 & \text{for } \begin{cases} j \in \{1, \dots, (\frac{p^k-1}{2})\} & \text{if } p \neq 2 \\ j \in \{1, \dots, (\frac{p^k}{2})\} & \text{if } p = 2 \end{cases} \\ P^{0,i} = -\sum_{j=2}^{p^k} P_{i+1,j} & \text{for } i \in \{0, \dots, (p^k - 1)\} \end{pmatrix} \right\} \tag{149}$$

is a differentiable manifold stemming from $\mathbf{vec}_{\mathbb{R}}(F_{p^k})$, and is generated, through $V \rightarrow \mathbf{vec}_{\mathbb{R}}(V)$, by unitary complex Hadamard matrices V dephased with respect to F_{p^k} according to $\mathcal{I}_{F_{p^k}}$ associated with $\mathcal{S}_{F_{p^k}}$.

We omit the proof, leaving the reader only with a sketch of it. Precise proofs of Theorem 6.1 and Theorem 6.2 can be found in the preprint version of this article [33].

Basing on the assumption that the matrix P satisfies the stated constraints:

- We first check that $F_{p^k} \circ \mathbf{EXP}(iP F_{p^k})$ is indeed dephased with respect to F_{p^k} .
- Next we show that $P F_{p^k} \in \mathcal{R}_{F_{p^k}}$, a linear subspace of real $p^k \times p^k$ matrices, defined in the following Theorem 6.2, presenting another construction of the considered family. This property guarantees that $F_{p^k} \circ \mathbf{EXP}(iP F_{p^k})$ is also unitary.
- Finally we parametrize the real space of the allowed $P F_{p^k}$ with the remaining $\mathbf{d}(F_{p^k})$ independent parameters left in P , to obtain a manifold parametrization for the set (149). This is a manifold around any of its points, and the above mentioned parametrization is a proper manifold parametrization for any values of the parameters.

Another construction of the discussed $\mathbf{d}(F_{p^k})$ dimensional family stemming from F_{p^k} is presented in the theorem below. However, the way in which the free parameters (phases) are scattered around a member matrix of the family seems to be more sophisticated in comparison with the pattern of parameters in a PCM matrix of the previous theorem.

Theorem 6.2. *Let, for p prime and $k \in \mathbb{N}$ such that $k > 1$, $\mathcal{R}_{F_{p^k}}$ be the set of all real $p^k \times p^k$ matrices R satisfying the independent constraints (where $\Delta_l^{i,j}$ denotes the difference $R_{i,l} - R_{j,l}$):*
the constraints of order $p^0 = 1$:

$$\Delta_l^{i,i+1} = \Delta_{l+p^{k-1}}^{i,i+1} = \Delta_{l+2p^{k-1}}^{i,i+1} = \dots = \Delta_{l+(p-1)p^{k-1}}^{i,i+1} \tag{150}$$

for $l = 1, 2, \dots, p^{k-1}$, and for $i \in \{1, 2, \dots, (p^k - 1)\}$ (one p^k -element cycle of differences of rows, counting $\Delta_{\dots}^{p^k,1}$).

the constraints of order p :

$$\Delta_l^{i,i+p} = \Delta_{l+p^{k-2}}^{i,i+p} = \Delta_{l+2p^{k-2}}^{i,i+p} = \dots = \Delta_{l+(p-1)p^{k-2}}^{i,i+p} \tag{151}$$

for $l = 1, 2, \dots, p^{k-2}$, and for $i \in \bigcup_{r \in \{1, \dots, p\}} \{r + sp : s \in \{0, 1, \dots, (p^{k-1} - 2)\}\}$ (p p^{k-1} -element cycles of differences, counting final wrappings).

the constraints of order p^2 :

$$\Delta_l^{i,i+p^2} = \Delta_{l+p^{k-3}}^{i,i+p^2} = \Delta_{l+2p^{k-3}}^{i,i+p^2} = \dots = \Delta_{l+(p-1)p^{k-3}}^{i,i+p^2} \tag{152}$$

for $l = 1, 2, \dots, p^{k-3}$, and for $i \in \bigcup_{r \in \{1, \dots, p^2\}} \{r + sp^2 : s \in \{0, 1, \dots, (p^{k-2} - 2)\}\}$ (p^2 p^{k-2} -element cycles of differences).

...

the constraints of order p^m :

$$\Delta_l^{i,i+p^m} = \Delta_{l+p^{k-(m+1)}}^{i,i+p^m} = \Delta_{l+2p^{k-(m+1)}}^{i,i+p^m} = \dots = \Delta_{l+(p-1)p^{k-(m+1)}}^{i,i+p^m} \tag{153}$$

for $l = 1, 2, \dots, p^{k-(m+1)}$, and for $i \in \bigcup_{r \in \{1, \dots, p^m\}} \{r + sp^m : s \in \{0, 1, \dots, (p^{k-m} - 2)\}\}$ (p^m p^{k-m} -element cycles of differences).

...

the constraints of order p^{k-1} :

$$\Delta_1^{i,i+p^{k-1}} = \Delta_2^{i,i+p^{k-1}} = \Delta_3^{i,i+p^{k-1}} = \dots = \Delta_p^{i,i+p^{k-1}} \tag{154}$$

for $i \in \bigcup_{r \in \{1, \dots, p^{k-1}\}} \{r + sp^{k-1} : s \in \{0, 1, \dots, (p-2)\}\}$ (p^{k-1} p -element cycles of differences).

the dephasing constraints:

$$R_{1,1} = R_{2,1} = \dots = R_{p^k,1} = R_{1,2} = R_{1,3} = \dots = R_{1,p^k} = 0 \tag{155}$$

Then $\mathcal{R}_{F_{p^k}}$ is a $\mathbf{d}(F_{p^k}) = p^{k-1}((k-1)p - k) + 1$ dimensional subspace of real $p^k \times p^k$ matrices, and if $R^{(1)}, R^{(2)}, \dots, R^{(\mathbf{d}(F_{p^k}))}$ form a basis of $\mathcal{R}_{F_{p^k}}$, then

$$\{\mathcal{F}(\phi_1, \dots, \phi_{\mathbf{d}(F_{p^k})}) : \phi_i \in \mathbb{R}\}, \tag{156}$$

where

$$\mathcal{F}(\phi_1, \dots, \phi_{\mathbf{d}(F_{p^k})}) = \mathbf{vec}_{\mathbb{R}} \left(F_{p^k} \circ \mathbf{EXP} \left(\mathbf{i} \sum_{i=1}^{\mathbf{d}(F_{p^k})} \phi_i \cdot R^{(i)} \right) \right) \tag{157}$$

is a $\mathbf{d}(F_{p^k})$ dimensional manifold (around $\mathbf{vec}_{\mathbb{R}}(F_{p^k})$) generated by dephased, with respect to F_{p^k} , unitary complex Hadamard matrices, stemming from $\mathbf{vec}_{\mathbb{R}}(F_{p^k})$, parametrized by function \mathcal{F} given by (157).

Again we omit the proof, providing only this sketch:

- We first check that $F_{p^k} \circ \mathbf{EXP}(\mathbf{i}R)$ is unitary for any $R \in \mathcal{R}_{F_{p^k}}$.
- We observe that all the constraints defining $\mathcal{R}_{F_{p^k}}$ must be independent, for otherwise the dimension of (156) would exceed the bound of Theorem 4.7. Thus $\mathcal{R}_{F_{p^k}}$ and (156) must be of dimension $\mathbf{d}(F_{p^k})$. (156) is a manifold around any of its points, and (157) is a proper manifold parametrization for any values of the parameters.

As examples, let us examine the $\mathbf{d}(F_N)$ -dimensional families stemming from $\mathbf{vec}_{\mathbb{R}}(F_{2^3})$ and $\mathbf{vec}_{\mathbb{R}}(F_{3^2})$. We present both forms, featured in Theorems 6.1 and 6.2, of these.

$$\begin{aligned} \mathcal{F}_{F_8}(a, b, c, d, e) &= \{\mathbf{vec}_{\mathbb{R}}(F_8 \circ \mathbf{EXP}(\mathbf{i} \cdot P_8(a, b, c, d, e) \cdot F_8)) : a, b, c, d, e \in \mathbb{R}\} \\ &= \{\mathbf{vec}_{\mathbb{R}}(F_8 \circ \mathbf{EXP}(\mathbf{i} \cdot R_8(a, b, c, d, e))) : a, b, c, d, e \in \mathbb{R}\}, \end{aligned} \tag{158}$$

where

$$P_8(a, b, c, d, e) = \left[\begin{array}{c|ccccccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -(2a+c) & 0 & (a+ib) & 0 & c & 0 & (a-ib) \\ -d & 0 & 0 & 0 & d & 0 & 0 \\ -(2a+e) & 0 & (a+ib) & 0 & e & 0 & (a-ib) \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -(2a+c) & 0 & (a+ib) & 0 & c & 0 & (a-ib) \\ -d & 0 & 0 & 0 & d & 0 & 0 \\ -(2a+e) & 0 & (a+ib) & 0 & e & 0 & (a-ib) \end{array} \right] \tag{159}$$

and

$$R_8(a, b, c, d, e) = \left[\begin{array}{cccc|cccc} \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & a & b & c & \bullet & a & b & c \\ \bullet & d & \bullet & d & \bullet & d & \bullet & d \\ \bullet & e & b & c - a + e & \bullet & e & b & c - a + e \\ \hline \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & a & b & c & \bullet & a & b & c \\ \bullet & d & \bullet & d & \bullet & d & \bullet & d \\ \bullet & e & b & c - a + e & \bullet & e & b & c - a + e \end{array} \right], \tag{160}$$

$$\begin{aligned} \mathcal{F}_{F_9}(a, b, c, d) &= \{\mathbf{vec}_{\mathbb{R}}(F_9 \circ \mathbf{EXP}(\mathbf{i} \cdot P_9(a, b, c, d) \cdot F_9)) : a, b, c, d \in \mathbb{R}\} \\ &= \{\mathbf{vec}_{\mathbb{R}}(F_9 \circ \mathbf{EXP}(\mathbf{i} \cdot R_9(a, b, c, d))) : a, b, c, d \in \mathbb{R}\}, \end{aligned} \tag{161}$$

where

$$P_9(a, b, c, d) = \left[\begin{array}{cccc|cccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -2a & 0 & 0 & (a + \mathbf{i}b) & 0 & 0 & (a - \mathbf{i}b) & 0 \\ -2c & 0 & 0 & (c + \mathbf{i}d) & 0 & 0 & (c - \mathbf{i}d) & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -2a & 0 & 0 & (a + \mathbf{i}b) & 0 & 0 & (a - \mathbf{i}b) & 0 \\ -2c & 0 & 0 & (c + \mathbf{i}d) & 0 & 0 & (c - \mathbf{i}d) & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -2a & 0 & 0 & (a + \mathbf{i}b) & 0 & 0 & (a - \mathbf{i}b) & 0 \\ -2c & 0 & 0 & (c + \mathbf{i}d) & 0 & 0 & (c - \mathbf{i}d) & 0 \end{array} \right] \tag{162}$$

and

$$R_9(a, b, c, d) = \left[\begin{array}{ccc|ccc|ccc} \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & a & b & \bullet & a & b & \bullet & a & b \\ \bullet & c & d & \bullet & c & d & \bullet & c & d \\ \hline \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & a & b & \bullet & a & b & \bullet & a & b \\ \bullet & c & d & \bullet & c & d & \bullet & c & d \\ \hline \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & a & b & \bullet & a & b & \bullet & a & b \\ \bullet & c & d & \bullet & c & d & \bullet & c & d \end{array} \right]. \tag{163}$$

Reasoning very much like in the proof of Theorem 4.2, one can prove the fact stated below about the discussed continuous families stemming from F_{p^k} . By 'dephased' matrices we mean dephased with respect to F_{p^k} in the manner described in the introductory part of this section.

Theorem 6.3. *There exists a neighbourhood \mathcal{W} of $\mathbf{vec}_{\mathbb{R}}(F_{p^k})$ in $\mathbb{R}^{2(p^k)^2}$ such that the only vectors $v \in \mathcal{W} \setminus \{\mathbf{vec}_{\mathbb{R}}(F_{p^k})\}$ generated by dephased unitary complex Hadamard matrices:*

$$v = \mathbf{vec}_{\mathbb{R}}(F_{p^k} \circ \mathbf{EXP}(\mathbf{i}R)), \quad \text{where } R_{1,j} = R_{i,1} = 0, \quad i, j \in \{1, \dots, p^k\}, \tag{164}$$

are those generated by the matrix forms of members of the continuous $\mathbf{d}(F_{p^k})$ -dimensional family of Theorem 6.2:

$$\{F_{p^k} \circ \mathbf{EXP}(\mathbf{i}R) : R \in \mathcal{R}_{F_{p^k}}\}, \tag{165}$$

where $\mathcal{R}_{F_{p^k}}$ is the $\mathbf{d}(F_{p^k})$ -dimensional linear space defined in Theorem 6.2.

Proof. Unitarity of $\mathbf{vec}_{\mathbb{R}}^{-1}(v) = F_{p^k} \circ \mathbf{EXP}(\mathbf{i}R)$ (see (164)) and the dephasing condition can be expressed, for $\mathbf{vec}(R) \in \mathbb{R}^{(p^k)^2}$, as the system of equations:

$$\begin{cases} R_{1,j} = 0, & j \in \{2, \dots, p^k\}, \\ R_{i,1} = 0, & i \in \{1, \dots, p^k\}, \\ g(\mathbf{vec}(R)) = \mathbf{0}, \end{cases} \tag{166}$$

where g is defined at the end of Section 2.2 in (38), and where U is taken to be F_{p^k} . The collective system will be denoted by

$$h(\mathbf{vec}(R)) = \mathbf{0}. \tag{167}$$

Looking at the form of the differential of g at $\mathbf{0}$ (see (39) and the description there) we notice that the differential of h at $\mathbf{0}$ satisfies:

$$\dim(Dh_{\mathbf{0}}(\mathbb{R}^{(p^k)^2})) = (p^k)^2 - \mathbf{d}(F_{p^k}), \tag{168}$$

as $\mathbf{vec}(e_k e^T)$, $k = 1, \dots, p^k$ and $\mathbf{vec}(e_l^T)$, $l = 2, \dots, p^k$, spanning a part of the kernel of $Dg_{\mathbf{0}}$, are no longer in the kernel of $Dh_{\mathbf{0}}$.

Thus one can choose a $((p^k)^2 - \mathbf{d}(F_{p^k}))$ -equation subsystem of (167) with the full rank:

$$\tilde{h}(\mathbf{vec}(R)) = \mathbf{0}, \quad \text{where } \dim(D\tilde{h}_{\mathbf{0}}(\mathbb{R}^{(p^k)^2})) = (p^k)^2 - \mathbf{d}(F_{p^k}). \tag{169}$$

Therefore system (169) defines a $\mathbf{d}(F_{p^k})$ -dimensional manifold around $\mathbf{0}$, and this must be the $\mathbf{d}(F_{p^k})$ -dimensional linear space $\mathbf{vec}(\mathcal{R}_{F_{p^k}})$ with $\mathcal{R}_{F_{p^k}}$ defined in Theorem 6.2, for it satisfies (169).

If $v \in \mathcal{W}$ and $\mathbf{vec}_{\mathbb{R}}^{-1}(v)$ is a dephased unitary complex Hadamard matrix, then $\mathbf{vec}_{\mathbb{R}}^{-1}(v) = F_{p^k} \circ \mathbf{EXP}(\mathbf{i}R)$ for some $\mathbf{vec}(R)$ close to $\mathbf{0}$, and $\mathbf{vec}_{\mathbb{R}}(R)$ must satisfy (169), i.e. $R \in \mathcal{R}_{F_{p^k}}$. \square

7. Conclusions

In this work we proposed a definition of the defect of a unitary matrix of size N . This notion is shown to be useful while investigating certain properties of unitary matrices. Demonstrating that the defect of any Fourier matrix of a prime size is equal to zero we infer that in this case F_N is an isolated unitary complex Hadamard matrix. This result also allows us to prove that for prime dimensions there exists a unistochastic ball around the flat bistochastic matrix J_N .

A positive value of the defect of F_N for a composite N provides a direct upper bound for the dimension of an orbit of dephased (and thus locally \simeq -inequivalent) unitary complex Hadamard matrices. Already for $N = 6$ this bound, equal to 4, is larger than the dimension $D = 2$ of the largest orbit known, which may suggest that the list of known Hadamard matrices is incomplete.

The defect of any U may be expressed using the rank of certain matrix associated with U and computed numerically. Such computations were performed for several unitaries of size $N = 6$ belonging to the known families of inequivalent unitary complex Hadamard matrices. In all cases studied the defect was equal to $\mathbf{d}(F_6) = 4$, which provides a hint [29] that these families may be embedded inside an unknown orbit of dimension 4. This reasoning allows us to believe that the notion of the defect will be useful in further search for new families of (unitary) complex Hadamard matrices.

In this paper we presented two constructions of $\mathbf{d}(F_N)$ -dimensional smooth families of inequivalent complex Hadamard matrices which stem from the Fourier matrix F_N . These constructions

work for N being a power of a prime number. One of them involves the ‘parameter cycle matrices’, which proved to be useful in computing the defect $\mathbf{d}(F_N)$. The family of complex Hadamard matrices obtained in this way has a particularly nice form which is due to the symmetric structure of F_N , and it is closely related to the fact that F_N diagonalizes circulant matrices of size N . Analogous properties of orbits of inequivalent matrices stemming from Kronecker products of Fourier matrices need further investigations for other composite N which are not a power of prime.

The defect of a unitary matrix is related to the map (1) projecting the N^2 dimensional set of unitary matrices into the $(N - 1)^2$ dimensional set of unistochastic matrices. The actual value of the defect provides a kind of characterization of the space of unitary matrices and allows one to classify its elements. For a generic unitary matrix $\mathbf{d}(U) = 0$, while any deviation from this value for a given U confirms certain special properties of the analyzed matrix. For instance, we find that the defect of a generic real orthogonal matrix O_N of size $N > 2$ is positive and satisfies $\mathbf{d}(O_N) \geq (N - 1)(N - 2)/2$. Although we have some knowledge on the defect of unitary matrices with a Kronecker product structure, the general problem of characterizing the class of unitary matrices of size N with a fixed defect remains open.

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Appendix A. Notation

We shall adopt the following conventions:

$A \circ B$ denotes the Hadamard product of matrices A and B

$\mathbf{diag}(v)$ denotes an $N \times N$ diagonal matrix, for an N element vector or sequence v , such that $[\mathbf{diag}(v)]_{i,i} = v_i$

$\mathbf{EXP}(A)$ denotes the entrywise operation \exp on matrix A

\mathbf{Re} , \mathbf{Im} denote also the entrywise operations \mathbf{Re} , \mathbf{Im} on matrices

$A_{i_1:i_2, j_1:j_2}$ denotes a sub-matrix of matrix A

$$A_{i_1:i_2, j_1:j_2} = \begin{bmatrix} A_{i_1, j_1} & \cdots & A_{i_1, j_2} \\ \cdots & \cdots & \cdots \\ A_{i_2, j_1} & \cdots & A_{i_2, j_2} \end{bmatrix}$$

If $i_1 = i_2$ or $j_1 = j_2$ we write i_1 , j_1 instead of $i_1 : i_2$, $j_1 : j_2$, respectively.

e_k denotes the k th standard basis column vector

\mathbf{e} denotes a vertical vector $[1, 1, \dots, 1]^T$ filled all with ones

$\mathbf{vec}_{\mathbb{C}}(A)$ ($\mathbf{vec}(A)$) denotes the ‘row by row’ vertical complex (real) vector form of a complex (real) $N \times N$ matrix A :

$$\mathbf{vec}_{\mathbb{C}}(A) = [A_{1,1}, \dots, A_{1,N}, A_{2,1}, \dots, A_{2,N}, \dots, A_{N,1}, \dots, A_{N,N}]^T$$

We identify \mathbb{R}^k (\mathbb{C}^k) with the set of all real (complex) vertical $k \times 1$ vectors (matrices).

$\text{vec}_{\mathbb{R}}(A)$ denotes the ‘row by row’ vertical real vector form of a complex $N \times N$ matrix A :

$$\text{vec}_{\mathbb{R}}(A) = \begin{bmatrix} \text{Re}(\text{vec}_{\mathbb{C}}(A)) \\ \text{Im}(\text{vec}_{\mathbb{C}}(A)) \end{bmatrix}$$

$\text{span}_{\mathbb{C}}(S)$ ($\text{span}_{\mathbb{R}}(S)$) denotes a complex (real) linear space spanned by vectors from a set or columns of a matrix S

$\text{null}_{\mathbb{C}}(D)$ ($\text{null}_{\mathbb{R}}(D)$) denotes, for an operator or matrix D , the complex space $\{v \in \mathbb{C}^N : D(v) = \mathbf{0}\}$. (the real space $\{r \in \mathbb{R}^N : D(r) = \mathbf{0}\}$)

\mathcal{B} denotes the set of all real matrices with all row and column sums equal to 1, for a given size N ; this includes bistochastic matrices which contain non-negative entries only

\mathcal{U} denotes the set of all unitary matrices, for a given size N

α denotes the following function generating indices into a matrix

$$\alpha : \{(i, j) : 1 \leq i < j \leq N\} \longrightarrow \left\{ 1, 2, \dots, \frac{(N-1)N}{2} \right\}$$

such that

$$\begin{array}{c|c|c|c|c|c|c|c|c} (i, j) & (1, 2) & \cdots & (1, N) & (2, 3) & \cdots & (2, N) & \cdots & (N-1, N) \\ \alpha(i, j) & 1 & \cdots & N-1 & N & \cdots & 2N-3 & \cdots & \frac{(N-1)N}{2} \end{array}$$

(141).

Appendix B. Proof of Theorem 5.3 on alternate formulae for the defect of the Fourier matrix F_N (by Wojciech Słomczyński)

a. From Theorem 5.2 and from the symmetry relations

$$\sum_{l=1}^{\frac{N-1}{2}} \text{gcd}(N, l) = \frac{1}{2} \left(\sum_{l=1}^{N-1} \text{gcd}(N, l) \right)$$

for odd N , and

$$\sum_{l=1}^{\frac{N}{2}-1} \text{gcd}(N, l) = \frac{1}{2} \left(\sum_{l=1}^{N-1} \text{gcd}(N, l) - \frac{N}{2} \right)$$

for even N , we deduce (141).

b. From (141) we get

$$\begin{aligned} \mathbf{d}(F_N) &= 1 - 2N + \sum_{l=1}^N \text{gcd}(N, l) \\ &= 1 - 2N + \sum_{d|N} d \cdot |\{l : 1 \leq l \leq N \text{ and } \text{gcd}(l, N) = d\}| \\ &= 1 - 2N + \sum_{d|N} d \cdot |\{k : 1 \leq k \leq N/d \text{ and } \text{gcd}(k, N/d) = 1\}| \end{aligned}$$

$$\begin{aligned}
 &= 1 - 2N + \sum_{d|N} d \cdot \varphi(N/d) \\
 &= N \left(\sum_{d|N} \frac{d}{N} \varphi(N/d) - 2 \right) + 1 \\
 &= N \left(\sum_{d|N} \psi(N/d) - 2 \right) + 1 \\
 &= N (\psi_{\leq}(N) - 2) + 1,
 \end{aligned} \tag{170}$$

where φ is the Euler function [32, p. 158] given by:

$$\varphi(M) := |\{k : 1 \leq k \leq M \text{ and } \gcd(k, M) = 1\}|,$$

ψ is an arithmetic function defined by

$$\psi(M) := \varphi(M)/M,$$

and the Möbius inverse function ψ_{\leq} is given by:

$$\psi_{\leq}(M) := \sum_{d|M} \psi\left(\frac{M}{d}\right).$$

We shall show that

$$\psi_{\leq}(N) = \prod_{j=1}^n \left(1 + k_j - \frac{k_j}{p_j}\right) =: R(N). \tag{171}$$

To prove (171) it suffices to apply the Möbius inversion formula [32, p. 154]

$$\psi(N) := \sum_{d|N} \psi_{\leq}\left(\frac{N}{d}\right) \mu(d)$$

and to show that

$$\psi(N) := \sum_{d|N} R\left(\frac{N}{d}\right) \mu(d), \tag{172}$$

where μ is the Möbius function defined as

$$\mu(d) := \begin{cases} (-1)^s & d = \prod_{j=1}^s p_j, \text{ where } p_j (j = 1, \dots, s) \text{ are different primes,} \\ 0 & \text{otherwise.} \end{cases}$$

From the Euler formula [32, p. 158]

$$\psi(N) = \varphi(N)/N = \prod_{j=1}^n \left(1 - \frac{1}{p_j}\right)$$

we deduce that

$$\begin{aligned}
 \psi(N) &= \prod_{j=1}^n \left(1 - \frac{1}{p_j}\right) \\
 &= \sum_{b \in \{0,1\}^n} \prod_{j=1}^n \left(1 + k_j - b_j - \frac{k_j - b_j}{p_j}\right) (-1)^{b_j}
 \end{aligned}$$

$$\begin{aligned}
&= \sum_{b \in \{0,1\}^n} R \left(\prod_{j=1}^n p_j^{k_j - b_j} \right) (-1)^{\sum_{j=1}^n b_j} \\
&= \sum_{d|N} R \left(\frac{N}{d} \right) \mu(d),
\end{aligned}$$

which proves (172), and, in consequence, (171).

Now, formula (142) follows from (171) and (170).

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