Defect of a Kronecker product of unitary matrices

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Abstract

The generalized defect $\mathbf{D}(U)$ of a unitary $N \times N$ matrix U with no zero entries is the dimension of the real space of directions, moving into which from U we do not disturb the moduli $|U_{i,j}|$ as well as the Gram matrix U^*U in the first order. Then the defect $\mathbf{d}(U)$ is equal to $\mathbf{D}(U) - (2N-1)$, that is the generalized defect diminished by the dimension of the manifold $\{D_r U D_c \ : \ D_r, D_c \text{ unitary diagonal}\}$. Calculation of $\mathbf{d}(U)$ involves calculating the dimension of the space in $\mathbb{R}^{N^2}$ spanned by a certain set of vectors associated with U. We split this space into a direct sum, assuming that U is a Kronecker product of unitary matrices, thus making it easier to perform calculations numerically. Basing on this, we give a lower bound on $\mathbf{D}(U)$ (equivalently $\mathbf{d}(U)$), supposing it is achieved for most unitaries with a fixed Kronecker product structure. Also supermultiplicativity of $\mathbf{D}(U)$ with respect to Kronecker subproducts of U is shown.

Keywords: unitary matrix, kronecker product, tensor product, complex Hadamard matrix, doubly stochastic matrix, critical point

MSC-class: 51F25, 47A80, 15B34, 15B51, 58A05

1 Introduction

The paper is a sequel to [1] where the defect of a unitary matrix was introduced and investigated in a general case.

Let $U \in \mathcal{U}$, where by $\mathcal{U}$ we shall denote the set of all unitaries $N \times N$. Consider the problem: find all directions (complex matrices) guaranteeing no first order change of $|U_{i,j}|$ for all i, j when moving from U in such a direction, and at the same time no first order disturbance of unitarity of U. The first requirement implies that these directions are of the form $\mathbf{i}R \circ U$ where $\circ$ is the Hadamard product and R is a real matrix. The second means that the directions in question must belong to the space tangent, at U, to the N^2 dimensional manifold $\mathcal{U}$. This tangent space is the set $\{EU : \ E \text{ antihermitian}\}$ or, if one likes, $\{UF : \ F \text{ antihermitian}\}$.

Note that the set of directions in question forms a real linear space and it is overparameterized by R in the case of U having zeros among its entries. If $U_{i,j} = 0$ then the equality $\mathbf{i}(R+\alpha e_i(e_j)^T) \circ U \ = \ \mathbf{i}R \circ U$, with e_k being the standard basis column vectors, exposes the fact that two different R's can be used to parameterize any single direction. Having this in mind we thus concentrate on the space of $R's$ parameterizing the space of directions in question:

$$\{R \ : \quad \mathbf{i}R \circ U \quad = \quad EU \quad \text{for some antihermitian } E\} \tag{1}$$

and ask about its dimension. We define the **defect** of U as this dimension diminished by $2N-1$.

If U has no zero entries, the defect plus $2N-1$ is precisely the dimension of the space of directions in question. The reduction by $2N-1$ is motivated by applications of the notion of defect. For most unitaries, especially those with no zero entries, the $2N$ directions:

$$\begin{aligned} \mathbf{i}\ e_i(\mathbf{e})^T \circ U &= \mathbf{i}\ \mathbf{diag}(e_i) \cdot U \qquad \text{for} \quad i = 1..N, \\ \mathbf{i}\ \mathbf{e}(e_j)^T \circ U &= U \cdot \mathbf{i}\ \mathbf{diag}(e_i) \qquad \text{for} \quad j = 1..N, \\ \text{where} \quad \mathbf{e} &= ([1\ 1\ 1\ \ldots 1])^T \end{aligned} \tag{2}$$

which are also directions in question, span the $2N-1$ dimensional real space tangent to the **phasing manifold** $\{D_r U D_c : \ D_r, D_c \text{ unitary diagonal}\}$ generated by left and right multiplication of U by unitary diagonals. The manifold consists of what we regard as unitaries **equivalent** to U, with the property of having moduli of entries identical with those of U. Usually the directions (2), leading from U to these equivalent unitaries, are uninteresting.

Other directions in question may lead to unitaries inequivalent to U, but with the same pattern of moduli, provided they exist in a neighbourhood of U. A special case of this property is the existence of a smooth family of inequivalent complex Hadamard matrices stemming from a given complex Hadamard matrix H. Here by a complex Hadamard matrix we understand, unlike in combinatorics community, a unitary with all moduli equal to $1/\sqrt{N}$, although matrices rescaled to have unimodular entries are more often considered in this context. As far as such complex Hadamard matrices are concerned, they have many applications especially in quantum information theory. We recommend the reader to consult the online catalogue of complex Hadamard matrices available at [3].

The smallest matrix size for which the known collection of inequivalent complex Hadamards is presumably incomplete is 6. Current investigations are concentrated on the search for a 4-dimensional smooth family of inequivalent complex Hadamards. This search is partly motivated by the fact that the value of the defect calculated for most known 6×6 complex Hadamards, including the unitary Fourier matrix F_6, is equal to 4. This is because the defect of a complex Hadamard H provides an upper bound for the dimension of a smooth family of inequivalent complex Hadamards stemming from H. We suggest the reader to throw a look into our previous work [1] to find more details about this application of the defect. There he can also find that the defect of unitary U (complex Hadamard H) being equal to zero implies that there are no unitaries (complex Hadamards) inequivalent to U (H) in its neighbourhood. At this point it is worth to recall that analogous (see [1]) result was obtained by Remus Nicoara in his work [4], under the name of 'span condition', but in a different context of commuting squares of algebras, in which complex Hadamard matrices are used to define commuting squares of matrix algebras.

This above mentioned value 4, as we now understand, causes one to suppose that all these 6×6 complex Hadamards (or complex Hadamards equivalent to these) with such a defect are connected by a single 4-dimensional family. The old 2-dimensional family stemming from the Fourier F_6 was reported, (among other even earlier sources [5, 6]) already in our catalogue [7, 3]. Other 1-dimensional families were constructed in [8, 9], 2-dimensional in [10, 11], 3 dimensional in [12], and the first attempt to build a 4-dimensional family of 6×6 inequivalent Hadamards has to be attributed to Ferenc Szöllősi due to his succesful work [13], inspired also by some numerical evidence of the existence of such a family contained in [14].

From the above collection of results we conclude that it is of value to study the notion of defect, to search for effective ways to calculate it or estimate it for unitary matrices of a large size.

In the following we employ another, more expedient characterization of the defect. To this end let us start with rewriting the definition (1),

$$\begin{aligned} \mathbf{i}R\circ U \quad = \quad EU \quad \text{for some antihermitian } E &\iff \\ (\mathbf{i}R\circ U)(U)^{*} \quad \text{is antihermitian} &\iff \\ U(R\circ U)^{*} \quad = \quad (R\circ U)(U)^{*} \quad , & \end{aligned} \tag{3}$$

where * denotes the Hermitian conjugate.

This further leads to

$$\begin{aligned} \forall\ 1\le i\le j\le N \quad [U]_{i,:}\left[\mathbf{diag}([R]_{j,:})\right]\left([U]_{j,:}\right)^{*} \quad &= \quad [U]_{i,:}\left[\mathbf{diag}([R]_{i,:})\right]\left([U]_{j,:}\right)^{*} \\ &\Updownarrow \\ \forall\ 1\le i< j\le N \quad [U]_{i,:}\left[\mathbf{diag}([R]_{j,:})\right]\left([U]_{j,:}\right)^{*} \quad &= \quad [U]_{i,:}\left[\mathbf{diag}([R]_{i,:})\right]\left([U]_{j,:}\right)^{*} \quad , \end{aligned} \tag{4}$$

where by $[X]_{k,:}$ the k-th row of X is denoted, we adopt MATLAB notation for rows and columns.

The above can be rewritten as

$$\forall\ 1\le i<j\le N \quad \mathbf{tr}R\left(M_U^{(i,j)}\right)^{T} \quad = \quad 0 \quad , \tag{5}$$

where

$$M_U^{(i,j)} = \left[\begin{array}{c} \cdots \ 0 \ \cdots \\ \vdots \\ [U]_{i,:} \circ \overline{[U]_{j,:}} \\ \vdots \\ \cdots \ 0 \ \cdots \\ \vdots \\ - [U]_{i,:} \circ \overline{[U]_{j,:}} \\ \vdots \\ \cdots \ 0 \ \cdots \end{array} \right] \begin{array}{c} \\ \\ i \\ \\ \\ \\ j \\ \\ \\ \end{array} = A_U^{(i,j)} + \mathbf{i} \cdot S_U^{(i,j)} \tag{6}$$

has only its i-th and j-th rows potentially filled with nonzeros. Here $A_U^{(i,j)}$ and $S_U^{(i,j)}$ denote the real and imaginary part of $M_U^{(i,j)}$.

Let us convert (5) into purely real conditions:

$$\forall\ 1 \le i < j \le N \qquad \mathbf{tr} R\left(A_U^{(i,j)}\right)^T = 0 \qquad \text{and} \qquad \mathbf{tr} R\left(S_U^{(i,j)}\right)^T = 0 \ , \tag{7}$$

The form $\mathbf{tr} A(B)^T$ is a Hilbert-Schmidt type inner product on the space of real $N \times N$ matrices, hence (7) amounts to orthogonality conditions in this space. Consequently, and in accordance with our initial definition the defect of U can be calculated as

$$\begin{aligned} & \dim\left(\{R :\ \mathbf{i} R \circ U = EU \quad \text{for some antihermitian } E\}\right) - (2N-1) \\ &= \dim\left(\left(\mathbf{span}\left(\left\{ A_U^{(i,j)},\ S_U^{(i,j)} \ :\ 1 \le i < j \le N \right\} \right) \right)^{\perp} \right) - (2N-1) \end{aligned} \tag{8}$$

where $()^{\perp}$ is used to indicate the orthogonal complement of the space $\mathbb{M}_U$ spanned by matrices $A_U^{(i,j)}$, $S_U^{(i,j)}$, i.e.,

$$\mathbb{M}_U \stackrel{def}{=} \mathbf{span}\left(\mathcal{M}_U\right) \ , \tag{9}$$

where,

$$\mathcal{M}_U \stackrel{def}{=} \left\{ A_U^{(i,j)} :\ 1 \le i < j \le N \right\} \cup \left\{ S_U^{(i,j)} :\ 1 \le i < j \le N \right\} \ , \tag{10}$$

The properties of orthogonal complements allow now for the following alternative definition of the defect:

Definition 1.1 *The defect of a unitary $N \times N$ matrix U is the number*

$$\begin{aligned} \mathbf{d}(U) &= \dim\left((\mathbb{M}_U)^{\perp} \right) - (2N-1) \\ &= (N-1)^2 - \dim\left(\mathbb{M}_U\right) \ . \end{aligned} \tag{11}$$

It was shown by Karabegov [2] that the set of those U for which the defect is greater than 0 is of the Haar measure zero within the set of all unitaries $N \times N$. In this article we give a lower bound on the defect of a Kronecker product of unitary matrices:

$$U \quad = \quad U^{(1)} \otimes U^{(2)} \otimes \ldots \otimes U^{(r)} \quad , \tag{12}$$

where the unitaries are of size $n_1 \times n_1$, $n_2 \times n_2$, ..., $n_r \times n_r$, respectively. The bound computed according to our formulas agrees with the defect obtained numerically for Kronecker products of random unitary matrices drawn according to the Haar measure on the unitary group.

However, we do not have here a result concerning measures, analogous to that of Karabegov. Namely, that for unitary matrices $U^{(k)}$ lying beyond a certain set of the Haar measure zero, within the set of all unitary $n_k \times n_k$ matrices, the defect of the resulting Kronecker product (12) is equal to our bound.

Note that the above Kronecker product structure forms a key tool in studying quantum composite systems. For instance, any local unitary operation acting on a system composed of r particles has the form (12). Thus our results on the defect describe algebraic properties of generic local unitary operations, which are also called quantum gates.

2 Preparation

Let us introduce vector indices into Kronecker product (12),

$$[U]_{[i_1..i_r],[j_1..j_r]} \stackrel{def}{=} U_{i,j} \quad , \tag{13}$$

where

$$i \quad = \quad (i_1 - 1)\prod_{k=2}^{r} n_k \quad + \quad (i_2 - 1)\prod_{k=3}^{r} n_k \quad + \quad \ldots \quad (i_{r-1} - 1)n_r \quad + \quad i_r \tag{14}$$

$$j \quad = \quad (j_1 - 1)\prod_{k=2}^{r} n_k \quad + \quad (j_2 - 1)\prod_{k=3}^{r} n_k \quad + \quad \ldots \quad (j_{r-1} - 1)n_r \quad + \quad j_r \tag{15}$$

and

$$[U]_{[i_1..i_r],[j_1..j_r]} \quad = \quad \left[U^{(1)}\right]_{i_1,j_1} \cdot \left[U^{(2)}\right]_{i_2,j_2} \cdot \ldots \cdot \left[U^{(r)}\right]_{i_r,j_r} \tag{16}$$

In the following, if not stated otherwise, i, j will correspond to the vector indices $[i_1..i_r]$, $[j_1..j_r]$.

Let us try for a while to understand vector indices better. The relation between ordinary and vector indices could be defined in a different, but completely equivalent way. For two distinct elements in $\{1..n_1\} \times \ldots \times \{1..n_r\}$ let us introduce a relation:

$$[i_1..i_r] \; < \; [j_1..j_r] \quad \Longleftrightarrow \quad i_1 = j_1, \; \ldots, \; i_p = j_p, \; i_{p+1} < j_{p+1} \;\; \text{for some} \;\; p \in \{1,..,r-1\} \quad . \tag{17}$$

Then the relation between ordinary indices and vector indices we choose to be the only bijection ϕ from $\{1,\ldots,\prod_{l=1}^{r} n_l\}$ into $\{1..n_1\} \times \ldots \times \{1..n_r\}$ (for which we write $\phi(i) = [i_1..i_r]$), which satisfies: $i < j \implies \phi(i) < \phi(j)$.

Later in this article we talk about subrows and submatrices, built from elementary objects (entries of a row for a subrow, rows or columns of a matrix for a submatrix) indexed by those i, whose k-th subindex i_k is fixed at some value: $i \in \mathcal{A} = \{i : i_k = \alpha\}$. Any $i \in \mathcal{A}$ is therefore determined by an element of $\{1..n_1\} \times \ldots \times \{1..n_{k-1}\} \times \{1..n_{k+1}\} \times \ldots \times \{1..n_r\}$, namely the reduced vector index $[i_1..i_{k-1}, i_{k+1}..i_r]$ being a subvector of $[i_1..i_{k-1}, \alpha, i_{k+1}..i_r]$ corresponding to i. We can introduce the relation $<$ for the reduced vector indices, and then we note that:

$$[i_1..i_{k-1}, i_{k+1}..i_r] < [j_1..j_{k-1}, j_{k+1}..j_r] \iff [i_1..i_{k-1}, \alpha, i_{k+1}..i_r] < [j_1..j_{k-1}, \alpha, j_{k+1}..j_r] \quad . \tag{18}$$

Ordering the reduced vector indices induces, again, their relation with reduced ordinary indices $i', j' \in \{1, \ldots, \prod_{l=1, l\neq k}^{r} n_l\}$ uniquely, that is it is the same as if we used appropriate versions of formulas (14), (15).

Let us analyze, as an example, the case of a submatrix A' of matrix A of size $N \times N$, $N = \prod_{l=1}^{r} n_l$. Let A' be built from rows of A indexed by $i \in \mathcal{A}$, with the order of rows preserved as is the habit when taking submatrices. Because for i, j indexing rows of A used to build A' and for i', j' corresponding to reduced vector indices for i and j there holds:

$$\begin{aligned} i < j \iff [i_1..i_{k-1}, \alpha, i_{k+1}..i_r] < [j_1..j_{k-1}, \alpha, j_{k+1}..j_r] \iff \\ [i_1..i_{k-1}, i_{k+1}..i_r] < [j_1..j_{k-1}, j_{k+1}..j_r] \iff i' < j' \\ \text{where } i', j' \in \{1, \ldots, \textstyle\prod_{l=1, l\neq k}^{r} n_l\} \end{aligned} \tag{19}$$

it is justified to say that the m-th row of A forming A' is the m'-th row of A'. Here m' is obtained from m in the composition of relations: $m \longrightarrow [m_1..m_{k-1}, \alpha, m_{k+1}..m_r] \longrightarrow [m_1..m_{k-1}, m_{k+1}..m_r] \longrightarrow m'$. Equivalently we could say that the $[m_1..m_{k-1}, \alpha, m_{k+1}..m_r]$-th row of matrix A is the $[m_1..m_{k-1}, m_{k+1}..m_r]$-th row of its submatrix A'.

Now we return to the main course of this lecture. From now on we silently assume that all Kronecker factors in (12) are of size at least 2. This we do for convenience of thinking, though we do not exclude the possibility that some or even all of the below arguments remain correct without this assumption. We will address this issue later after announcing the main results at the end of this and at the beginning of the next section.

Using the introduced vector indices, we will split set $\mathcal{M}_U$ defined in (10) into disjoint subsets $(\mathcal{M}_U)_{(k_1,k_2,..,k_p),(v_1,v_2,..,v_p)}$,

Definition 2.1

$$(\mathcal{M}_U)_{(k_1,k_2,..,k_p),(v_1,v_2,..,v_p)} \quad = \tag{20}$$

$$\left\{ A_U^{(i,j)},\ S_U^{(i,j)} \ : \ \begin{array}{rcl} i_{k_1} = j_{k_1} & = & v_1 \in \{1..n_{k_1}\} \\ i_{k_2} = j_{k_2} & = & v_2 \in \{1..n_{k_2}\} \\ & \ldots & \\ i_{k_p} = j_{k_p} & = & v_r \in \{1..n_{k_p}\} \end{array} \ and \ \ i_k \ \neq \ j_k \ \ for \ \ k \in \{1..r\} \setminus \{k_1, k_2, .., k_p\} \right\} \ ,$$

where we assume that $1 \leq k_1 < \ldots < k_p \leq r, \quad 1 \leq p \leq r-1$, *and*

$$(\mathcal{M}_U)_{(),()} \quad = \quad \left\{ A_U^{(i,j)},\ S_U^{(i,j)} \ : \ \ i_1 \neq j_1,\ i_2 \neq j_2,\ \ldots,\ i_r \neq j_r \right\} \ , \tag{21}$$

where () *means the empty sequence of indices.*

The corresponding subspaces will be denoted according to the following

Definition 2.2

$$(\mathbb{M}_U)_{(),()} \ \stackrel{def}{=} \ \mathbf{span}\Big((\mathcal{M}_U)_{(),()} \Big) \tag{22}$$

$$(\mathbb{M}_U)_{(k_1,..,k_p),(v_1,..,v_p)} \ \stackrel{def}{=} \ \mathbf{span}\Big((\mathcal{M}_U)_{(k_1,..,k_p),(v_1,..,v_p)} \Big) \tag{23}$$

Note that in both of the above definitions the notation refers to the assumed Kronecker product structure of U. Later we will meet U deprived of one or more of its Kronecker factors. Accordingly, the resulting U' will be assumed to be built from a fewer number of factors, and this will be reflected in the notation used for subsets of $\mathcal{M}_{U'}$ and subspaces of $\mathbb{M}_{U'}$.

Any vector in $\mathbb{M}_U$ (see (9)) can be written as a linear combination of components each of which belongs to one of the above defined subspaces, hence $\mathbb{M}_U$ is the algebraic sum of all of them,

$$\begin{aligned} \mathbb{M}_U \quad = \quad & \\ & (\mathbb{M}_U)_{(),()} \ + \ \textstyle\sum_{k\in\{1..r\}} \sum_{v\in\{1..n_k\}} (\mathbb{M}_U)_{(k),(v)} \ + \\ & + \ \textstyle\sum_{k_1<k_2\in\{1..r\}} \sum_{(v_1,v_2)\in\{1..n_{k_1}\}\times\{1..n_{k_2}\}} (\mathbb{M}_U)_{(k_1,k_2),(v_1,v_2)} \ + \ \ldots \\ & \ldots \ + \ \textstyle\sum_{k_1<..<k_{r-1}\in\{1..r\}} \sum_{(v_1,..,v_{r-1})\in\{1..n_{k_1}\}\times..\times\{1..n_{k_{r-1}}\}} (\mathbb{M}_U)_{(k_1,..,k_{r-1}),(v_1,..,v_{r-1})} \end{aligned} \tag{24}$$

Our aim is to show that (24) is in fact a direct sum, which will allow to estimate its dimension. In the meantime a little preparation is needed.

Using notation similar to that of MATLAB, let, with y at the l-th position,

$$\begin{aligned} & [X]_{[i_1,..,i_r],[:,..,:,y,:,..,:]} \quad = \\ & \Big[[X]_{[i_1,..,i_r],[1,..,1,y,1,..,1,1]}, \ \ [X]_{[i_1,..,i_r],[1,..,1,y,1,..,1,2]}, \ \ \ldots, \ \ [X]_{[i_1,..,i_r],[n_1,..,n_{l-1},y,n_{l+1},..,n_{r-1},n_r]} \Big] \end{aligned} \tag{25}$$

be a subrow of the $[i_1,..,i_r]$-th row of matrix X of the size identical with the size of the Kronecker product (12). The subrow is composed of entries of $[j_1,..,j_r]$-th columns for which $j_l = y$. The horizontal order of entries is preserved.

Lemma 2.3 *Let $[i_1,..,i_r]$, $[j_1,..,j_r]$ be vector indices of the Kronecker product (12) corresponding to ordinary indices i,j.*

a) *If $i_k \neq j_k$ then any $[b_1,..,b_r]$-th row of $A_U^{(i,j)}$, $S_U^{(i,j)}$ satifies:*

$$\sum_{c_k=1}^{n_k} \left[A_U^{(i,j)}\right]_{[b_1,..,b_r],[:,..,:,c_k,:,..,:]} = \mathbf{0} \tag{26}$$

$$\sum_{c_k=1}^{n_k} \left[S_U^{(i,j)}\right]_{[b_1,..,b_r],[:,..,:,c_k,:,..,:]} = \mathbf{0} \tag{27}$$

where c_k is at the k-th position.

b) *If $i_k = j_k$ then*

$$\sum_{c_k=1}^{n_k} \left[A_U^{(i,j)}\right]_{[b_1,..,b_r],[:,..,:,c_k,:,..,:]} = \left[A_{U'}^{(i',j')}\right]_{[b_1,..,b_{k-1},b_{k+1},..,b_r],:} \tag{28}$$

$$\sum_{c_k=1}^{n_k} \left[S_U^{(i,j)}\right]_{[b_1,..,b_r],[:,..,:,c_k,:,..,:]} = \left[S_{U'}^{(i',j')}\right]_{[b_1,..,b_{k-1},b_{k+1},..,b_r],:} \tag{29}$$

for any $[b_1,..,b_r]$-th row such that $b_k = i_k = j_k$, c_k as above. On the right hand sides of (28) and (29) stand $[b_1,..,b_{k-1},b_{k+1},..,b_r]$-th rows of matrices $A_{U'}^{(i',j')}$, $S_{U'}^{(i',j')}$ constructed from the Kronecker product (12) deprived of its k-th factor:

$$U' = U^{(1)} \otimes \ldots \otimes U^{(k-1)} \otimes U^{(k+1)} \otimes \ldots \otimes U^{(r)} \quad . \tag{30}$$

Ordinary indices i', j' correspond to the accordingly reduced vector indices $[i_1,..,i_{k-1},i_{k+1},..,i_r]$, $[j_1,..,j_{k-1},j_{k+1},..,j_r]$.

Proof

a) is of course true for any row of $A_U^{(i,j)}$, $S_U^{(i,j)}$ indexed by a number different from i,j, which is in fact a zero row. As the i-th and j-th rows of $A_U^{(i,j)}$, $S_U^{(i,j)}$ are of opposite signs, we show **a)** only for the i-th row. We do it by proving that every element of the left hand side of (26) and (27) is equal to 0. Indeed for $M_U^{(i,j)}$ defined in (6) we have

$$\sum_{c_k=1}^{n_k} \left[M_U^{(i,j)}\right]_{[i_1,..,i_r],[c_1,..,c_r]} = \tag{31}$$

$$\sum_{c_k=1}^{n_k} \left([U]_{[i_1,..,i_r],[c_1,..,c_r]} \cdot \overline{[U]_{[j_1,..,j_r],[c_1,..,c_r]}}\right) =$$

$$\sum_{c_k=1}^{n_k} \left(\left[U^{(1)}\right]_{i_1,c_1} \cdot \ldots \cdot \left[U^{(r)}\right]_{i_r,c_r}\right) \cdot \left(\overline{\left[U^{(1)}\right]_{j_1,c_1}} \cdot \ldots \cdot \overline{\left[U^{(r)}\right]_{j_r,c_r}}\right) =$$

$$\left(\left[U^{(k)}\right]_{i_k,1}\overline{\left[U^{(k)}\right]_{j_k,1}} + \ldots + \left[U^{(k)}\right]_{i_k,n_k}\overline{\left[U^{(k)}\right]_{j_k,n_k}}\right) \cdot \prod_{l=1,\ l\neq k}^{r} \left(\left[U^{(l)}\right]_{i_l,c_l}\overline{\left[U^{(l)}\right]_{j_l,c_l}}\right) =$$

$$0 + 0\mathbf{i} \ ,$$

so its real and imaginary parts satisfy (26) and (27) respectively.

Now part **b)**. If $[b_1, .., b_r]$ satisfying $b_k = i_k = j_k$ is different from $[i_1, .., i_r]$, $[j_1, .., j_r]$, then the ordinary index b' corresponding to the reduced vector index $[b_1, .., b_{k-1}, b_{k+1}, .., b_r]$ is different from i', j'. In this situation both sides of (28), (29) are zero rows.

Next we consider the i-th row, $[b_1, .., b_r] = [i_1, .., i_r]$. Again, we investigate the sums (28) and (29) entrywise. As above, we have:

$$\sum_{c_k=1}^{n_k} \left[M_U^{(i,j)}\right]_{[i_1,..,i_r],[c_1,..,c_r]} = \tag{32}$$

$$\left(\left|\left[U^{(k)}\right]_{i_k,1}\right|^2 + \ldots + \left|\left[U^{(k)}\right]_{i_k,n_k}\right|^2\right) \cdot \prod_{l=1,\ l\neq k}^{r} \left(\left[U^{(l)}\right]_{i_l,c_l}\overline{\left[U^{(l)}\right]_{j_l,c_l}}\right) =$$

$$\left(\prod_{l=1,\ l\neq k}^{r} \left[U^{(l)}\right]_{i_l,c_l}\right) \cdot \overline{\left(\prod_{l=1,\ l\neq k}^{r} \left[U^{(l)}\right]_{j_l,c_l}\right)} =$$

$$[U']_{[i_1,..,i_{k-1},i_{k+1},..,i_r],[c_1,..,c_{k-1},c_{k+1},..,c_r]} \cdot \overline{[U']_{[j_1,..,j_{k-1},j_{k+1},..,j_r],[c_1,..,c_{k-1},c_{k+1},..,c_r]}} =$$

$$\left[M_{U'}^{(i',j')}\right]_{i',c'} \ ,$$

where the ordinary indices i', j', c' correspond to the vectors indices $[i_1, .., i_{k-1}, i_{k+1}, .., i_r]$, $[j_1, .., j_{k-1}, j_{k+1}, .., j_r]$, $[c_1, .., c_{k-1}, c_{k+1}, .., c_r]$ respectively. Now, by taking the real and imaginary part we get equalities (28) and (29). Calculations for the j-th row are completely analogous with the sign changed.

■

The properties stated in the above lemma extend to linear combinations of matrices $A_U^{(i,j)}$, $S_U^{(i,j)}$.

Lemma 2.4 *Let* $B \in (\mathbb{M}_U)_{(k_1,..,k_p),(v_1,..,v_p)}$. *Then:*

a) *For any* $k_s \in \{k_1, .., k_p\}$, *any* $c_{k_s} \in \{1..n_{k_s}\}$, *and any* $[b_1, .., b_r]$*-th row in* B*:*

$$[B]_{[b_1,..,b_r],[:,..,:,c_{k_s},:,..,:]} = \left|\left[U^{(k_s)}\right]_{v_s,c_{k_s}}\right|^2 \cdot \sum_{d_{k_s}=1}^{n_{k_s}} [B]_{[b_1,..,b_r],[:,..,:,d_{k_s},:,..,:]} \tag{33}$$

where c_{k_s}, d_{k_s} *both at* k_s*-th position designate subrows of row* $[B]_{[b_1,..,b_r],:}$.

In other words: the c_{k_s}*-th subrow is a multiple of the sum of all subrows designated by all the values of the* k_s*-th subindex.*

b) *For any* $k' \notin \{k_1..k_p\}$ *and any b-th row in B:*

$$\sum_{c_{k'}=1}^{n_{k'}} [B]_{b,[:,..,:,c_{k'},:,..,:]} = \mathbf{0} \qquad \text{where } c_{k'} \text{ is at } k'\text{-th position.} \tag{34}$$

Proof

The part **a)** of the lemma is of course true for all rows indexed by $[b_1, .., b_r]$ such that $b_{k_1} \neq v_1$ or $b_{k_2} \neq v_2$ or ... or $b_{k_p} \neq v_p$, since these are zero rows coming from zero rows in $A_U^{(i,j)}$, $S_U^{(i,j)}$ spanning $(\mathbb{M}_U)_{(k_1,..,k_p),(v_1,..,v_p)}$.

Let us thus consider the $[b_1, .., b_r]$-th row of B with $b_{k_1} = v_1$, $b_{k_2} = v_2$, ..., $b_{k_p} = v_p$. Since $B \in (\mathbb{M}_U)_{(k_1,..,k_p),(v_1,..,v_p)}$ for the $[b_1, .., b_r]$-th row we have,

$$\begin{aligned} [B]_{[b_1,..,b_r],:} \quad = & \\ \textstyle\sum_{A_U^{(i,j)} \in (\mathcal{M}_U)_{(k_1,..,k_p),(v_1,..,v_p)}} \alpha^{(i,j)} \left[A_U^{(i,j)}\right]_{[b_1,..,b_r],:} & \quad + \\ \textstyle\sum_{S_U^{(i,j)} \in (\mathcal{M}_U)_{(k_1,..,k_p),(v_1,..,v_p)}} \sigma^{(i,j)} \left[S_U^{(i,j)}\right]_{[b_1,..,b_r],:} & \quad , \end{aligned} \tag{35}$$

and analogously for the c_{k_s}-th subrow designated by the value of the k_s-th index, where we ommit the ranges for $\alpha^{(i,j)}$ and $\sigma^{(i,j)}$:

$$\begin{aligned} [B]_{[b_1,..,b_r],[:,..,:,c_{k_s},:,..,:]} \quad = & \\ \textstyle\sum_{....} \alpha^{(i,j)} \left[A_U^{(i,j)}\right]_{[b_1,..,b_r],[:,..,:,c_{k_s},:,..,:]} \quad + \quad \textstyle\sum_{....} \sigma^{(i,j)} \left[S_U^{(i,j)}\right]_{[b_1,..,b_r],[:,..,:,c_{k_s},:,..,:]} & \quad . \end{aligned} \tag{36}$$

Hence, on the one hand:

$$\begin{aligned} \sum_{d_{k_s}=1}^{n_{k_s}} [B]_{[b_1,..,b_r],[:,..,:,d_{k_s},:,..,:]} \quad = & \\ \textstyle\sum_{....} \alpha^{(i,j)} \sum_{d_{k_s}=1}^{n_{k_s}} \left[A_U^{(i,j)}\right]_{[b_1,..,b_r],[:,..,:,d_{k_s},:,..,:]} \quad + \quad \textstyle\sum_{....} \sigma^{(i,j)} \sum_{d_{k_s}=1}^{n_{k_s}} \left[S_U^{(i,j)}\right]_{[b_1,..,b_r],[:,..,:,d_{k_s},:,..,:]} & \quad = \\ \textstyle\sum_{....} \alpha^{(i,j)} \left[A_{U'}^{(i',j')}\right]_{[b_1,..,b_{k_s-1},b_{k_s+1},..,b_r],:} \quad + \quad \textstyle\sum_{....} \sigma^{(i,j)} \left[S_{U'}^{(i',j')}\right]_{[b_1,..,b_{k_s-1},b_{k_s+1},..,b_r],:} & \end{aligned} \tag{37}$$

where we used Lemma 2.3 **b)**, which can be employed since the indices i,j in the sums satisfy $i_{k_1} = j_{k_1} = v_1$, ..., $i_{k_p} = j_{k_p} = v_p$, and in particular $i_{k_s} = j_{k_s}$, as well as $b_{k_s} = v_s = i_{k_s} = j_{k_s}$. As previously, the ordinary indices i', j' correspond to vector indices

$[i_1, .., i_{k_s-1}, i_{k_s+1}, ..., i_r]$, $[j_1, .., j_{k_s-1}, j_{k_s+1}, ..., j_r]$ and designate nonzero rows in matrices $A_{U'}^{(i',j')}$, $S_{U'}^{(i',j')}$ constructed from the reduced Kronecker product $U^{(1)} \otimes .. \otimes U^{(k_s-1)} \otimes U^{(k_s+1)} \otimes .. \otimes U^{(r)}$.

On the other hand the expression (36) translates into

$$[B]_{[b_1,..,b_r],[:,..,:,c_{k_s},:,..,:]} = \sum\nolimits_{....} \alpha^{(i,j)} \left| \left[U^{(k_s)}\right]_{v_s,c_{k_s}} \right|^2 \left[A_{U'}^{(i',j')}\right]_{[b_1,..,b_{k_s-1},b_{k_s+1},..,b_r],:} + \sum\nolimits_{....} \sigma^{(i,j)} \left| \left[U^{(k_s)}\right]_{v_s,c_{k_s}} \right|^2 \left[S_{U'}^{(i',j')}\right]_{[b_1,..,b_{k_s-1},b_{k_s+1},..,b_r],:} , \tag{38}$$

with U', i', j' described above. Combining (37) and (38) we obtain **a)**.

To prove the part **b)** we use again (35) and rewrite it for the subrows corresponding to $k' \notin \{k_1..k_p\}$:

$$[B]_{[b_1,..,b_r],[:,..,:,c_{k'},:,..,:]} = \sum\nolimits_{....} \alpha^{(i,j)} \left[A_U^{(i,j)}\right]_{[b_1,..,b_r],[:,..,:,c_{k'},:,..,:]} + \sum\nolimits_{....} \sigma^{(i,j)} \left[S_U^{(i,j)}\right]_{[b_1,..,b_r],[:,..,:,c_{k'},:,..,:]} \tag{39}$$

Here i, j are such that $i_{k'} \neq j_{k'}$. We may thus use Lemma 2.3 **a)** to find that summation of subrows (39) produces a zero vector:

$$\sum_{c_{k'}=1}^{n_{k'}} [B]_{[b_1,..,b_r],[:,..,:,c_{k'},:,..,:]} = \sum\nolimits_{....} \alpha^{(i,j)} \sum\nolimits_{c_{k'}=1}^{n_{k'}} \left[A_U^{(i,j)}\right]_{[b_1,..,b_r],[:,..,:,c_{k'},:,..,:]} + \sum\nolimits_{....} \sigma^{(i,j)} \sum\nolimits_{c_{k'}=1}^{n_{k'}} \left[S_U^{(i,j)}\right]_{[b_1,..,b_r],[:,..,:,c_{k'},:,..,:]} = \sum\nolimits_{....} \alpha^{(i,j)} \cdot \mathbf{0} + \sum\nolimits_{....} \sigma^{(i,j)} \cdot \mathbf{0} = \mathbf{0} . \tag{40}$$

■

Related is the following result which we will also need to prove the theorem on a direct sum that comes next.

Lemma 2.5 *Let* $\left(\tilde{M}_U\right)_{k,v}$ *be the space spanned by matrices* $A_U^{(i,j)}$, $S_U^{(i,j)}$ *such that* $i_k = j_k = v$, *where* $v \in \{1..n_k\}$. *There exists an isomorphism mapping* $\left(\tilde{M}_U\right)_{k,v}$ *onto* $\mathbb{M}_{U'}$, *where* $U' = U^{(1)} \otimes \ldots \otimes U^{(k-1)} \otimes U^{(k+1)} \otimes \ldots \otimes U^{(r)}$. *It can be chosen in such a way that any subspace* $(\mathbb{M}_U)_{(k_1,..,k_p),(v_1,..,v_p)}$ *of* $\left(\tilde{M}_U\right)_{k,v}$ *with* $k_q = k$ *and* $v_q = v$ *for some* $q \in \{1..p\}$, *is mapped onto the subspace* $(\mathbb{M}_{U'})_{(k'_1,..,k'_{p-1}),(v_1,..,v_{q-1},v_{q+1},..v_p)}$ *of* $\mathbb{M}_{U'}$, *where* k'_1, ..., k'_{p-1} *are positions of* k_1, ..., k_{q-1}, k_{q+1}, ..., k_p *in the sequence* $(1, 2, ..., k-1, k+1, ..., r)$. *(Note that* k'_g *indicate positions of factors* $U^{(k_1)}$, ..., $U^{(k_{q-1})}$, $U^{(k_{q+1})}$, ..., $U^{(k_p)}$ *in the product* U'.*) In particular the chosen isomorphism maps* $(\mathbb{M}_U)_{(k),(v)}$ *onto* $(\mathbb{M}_{U'})_{(),()}$.

Proof

We will show that matrices $A_U^{(i,j)}$, $S_U^{(i,j)}$ spanning $\left(\tilde{M}_U\right)_{k,v}$ remain in a simple relation with matrices $A_{U'}^{(i',j')}$, $S_{U'}^{(i',j')}$. Here i', j' correspond to vector indices $[i_1,..,i_{k-1},i_{k+1},..,i_r]$, $[j_1,..,j_{k-1},j_{k+1},..,j_r]$ of the reduced Kronecker product U' (30), i.e., are given by the appropriate versions of (14) and (15).

We will be more precise about the above mentioned relation later, but at first let us state it without too many details. Any $A_U^{(i,j)}$ spanning $\left(\tilde{M}_U\right)_{k,v}$ contains, as its only nonzero and disjoint submatrices, n_k copies of the corresponding $A_{U'}^{(i',j')}$, where each copy is multiplied by one of n_k multipliers. Column positions of the copies do not depend on i, j. The multipliers, of which at least one is nonzero, depend only on the column positions of the copies they act on. The same applies to $S_U^{(i,j)}$ and $S_{U'}^{(i',j')}$, with the pattern of submatrices and values of the multipliers identical with that for $A_U^{(i,j)}$ and $A_{U'}^{(i',j')}$.

For a more detailed explanation let us consider the i-th row of $A_U^{(i,j)}$. The $[d_1,..,d_{k-1},d_{k+1},..,d_r]$-th element of the d_k-th subrow of it, $d_k \in \{1..n_k\}$, reads:

$$\left[A_U^{(i,j)}\right]_{i,[d_1,..,d_k,..,d_r]} = \mathbf{Re}\left(\left[M_U^{(i,j)}\right]_{i,[d_1,..,d_k,..,d_r]}\right) = \mathbf{Re}\left([U]_{i,[d_1,..,d_k,..,d_r]} \cdot \left[\overline{U}\right]_{j,[d_1,..,d_k,..,d_r]}\right) \quad , \tag{41}$$

which is equal to

$$\mathbf{Re}\left(\left[U^{(1)}\right]_{i_1,d_1}\left[\overline{U^{(1)}}\right]_{j_1,d_1} \cdot \ldots \cdot \left[U^{(k)}\right]_{i_k,d_k}\left[\overline{U^{(k)}}\right]_{j_k,d_k} \cdot \ldots \cdot \left[U^{(r)}\right]_{i_r,d_r}\left[\overline{U^{(r)}}\right]_{j_r,d_r}\right) \quad , \tag{42}$$

where $\left[U^{(k)}\right]_{i_k,d_k}\left[\overline{U^{(k)}}\right]_{j_k,d_k}$ can also be written as $\left[U^{(k)}\right]_{v,d_k}\left[\overline{U^{(k)}}\right]_{v,d_k} = \left|\left[U^{(k)}\right]_{v,d_k}\right|^2$. As a result we get

$$\left|\left[U^{(k)}\right]_{v,d_k}\right|^2 \cdot \mathbf{Re}\left(\prod_{s\in\{1..r\}\setminus k}\left[U^{(s)}\right]_{i_s,d_s}\left[\overline{U^{(s)}}\right]_{j_s,d_s}\right) = \tag{43}$$
$$\left|\left[U^{(k)}\right]_{v,d_k}\right|^2 \cdot \mathbf{Re}\left([U']_{[i_1,..,i_{k-1},i_{k+1},..,i_r],[d_1,..,d_{k-1},d_{k+1},..,d_r]} \cdot \left[\overline{U'}\right]_{[j_1,..,j_{k-1},j_{k+1},..,j_r],[d_1,..,d_{k-1},d_{k+1},..,d_r]}\right) =$$
$$\left|\left[U^{(k)}\right]_{v,d_k}\right|^2 \cdot \mathbf{Re}\left(\left[M_{U'}^{(i',j')}\right]_{i',[d_1,..,d_{k-1},d_{k+1},..,d_r]}\right) = \left|\left[U^{(k)}\right]_{v,d_k}\right|^2 \cdot \left[A_{U'}^{(i',j')}\right]_{i',[d_1,..,d_{k-1},d_{k+1},..,d_r]} \quad .$$

The equality of the far left hand side of (41) and the far right hand side of (43) is an entry by entry equality between two rows. Now, if we change the sign of **Re** in the expressions in (41), (42) and (43) we will obtain a relation between the d_k-th subrow of the j-th row in $A_U^{(i,j)}$ and the j'-th row of $A_{U'}^{(i',j')}$. If we used **Im** instead of **Re**, we would get a relation between the d_k-th subrow of the i-th or j-th row of $S_U^{(i,j)}$ and, correspondingly, the i'-th or j'-th row of $S_{U'}^{(i',j')}$. This is summarized below:

$$\begin{aligned}
\left[A_U^{(i,j)}\right]_{i,[:,..,:,d_k,:,..,:]} &= \mu_k \cdot \left[A_{U'}^{(i',j')}\right]_{i',:} , \\
\left[A_U^{(i,j)}\right]_{j,[:,..,:,d_k,:,..,:]} &= \mu_k \cdot \left[A_{U'}^{(i',j')}\right]_{j',:} , \\
\left[S_U^{(i,j)}\right]_{i,[:,..,:,d_k,:,..,:]} &= \mu_k \cdot \left[S_{U'}^{(i',j')}\right]_{i',:} , \\
\left[S_U^{(i,j)}\right]_{j,[:,..,:,d_k,:,..,:]} &= \mu_k \cdot \left[S_{U'}^{(i',j')}\right]_{j',:} ,
\end{aligned} \tag{44}$$

where $\mu_k = \left|\left[U^{(k)}\right]_{v,d_k}\right|^2$. One of the n_k numbers μ_k is nonzero since $U^{(k)}$ is unitary.

Now let us use $[X]_{[:,..,:,b_k,:,..,:],[:,..,:,c_k,:,..,:]}$ to denote a submatrix of X built of those x-th rows and y-th columns of X for which $x_k = b_k$ and $y_k = c_k$. As a consequence of relations (44) we see that $A_U^{(i,j)}$, $S_U^{(i,j)}$ spanning $\left(\tilde{M}_U\right)_{k,v}$ are all zero matrices except for their submatrices:

$$\left[A_U^{(i,j)}\right]_{[:,..,:,v,:,..,:],[:,..,:,c_k,:,..,:]} = \mu_k \cdot A_{U'}^{(i',j')} \qquad c_k \in \{1,..,n_k\} , \tag{45}$$

$$\left[S_U^{(i,j)}\right]_{[:,..,:,v,:,..,:],[:,..,:,c_k,:,..,:]} = \mu_k \cdot S_{U'}^{(i',j')} \qquad c_k \in \{1,..,n_k\} , \tag{46}$$

$$\text{where} \quad \mu_k = \left|\left[U^{(k)}\right]_{v,c_k}\right|^2$$

(where v is at k-th position), with one of μ_k being nonzero. Analogous equalities we could write for linear combinations on both sides. ((45) and (46) can be checked entry-wise, in which one uses that the $[b_1,..,b_{k-1},b_{k+1},..,b_r],[c_1,..,c_{k-1},c_{k+1},..,c_r]$-th element of $[X]_{[:,..,:,b_k,:,..,:],[:,..,:,c_k,:,..,:]}$ is equal to $[X]_{[b_1,..,b_r],[c_1,..,c_r]}$. Here of course we identify, for example, $[b_1,..,b_{k-1},b_{k+1},..,b_r]$ with ordinary index b'. See also the comment that follows the introduction of vector indices.)

Since all μ_k add up to 1 , i.e. the norm of the v-th row of $U^{(k)}$, we can choose an isomorphism Ψ between $\left(\tilde{M}_U\right)_{k,v}$ and $\mathbb{M}_{U'}$ to be defined as (again assuming that v stands at k-th position):

$$\Psi\left(X \in \left(\tilde{M}_U\right)_{k,v}\right) = \sum_{c_k=1}^{n_k} [X]_{[:,..,:,v,:,..,:],[:,..,:,c_k,:,..,:]} . \tag{47}$$

so that

$$\begin{aligned}
\Psi\left(A_U^{(i,j)}\right) &= A_{U'}^{(i',j')} \\
\Psi\left(S_U^{(i,j)}\right) &= S_{U'}^{(i',j')}
\end{aligned} \tag{48}$$

Consider now $(\mathbb{M}_U)_{(k_1,..,k_p),(v_1,..,v_p)} \subset \left(\tilde{M}_U\right)_{k,v}$ with $k_q = k$ and $v_q = v$ for some $q \in \{1,..,p\}$. Matrices $A_U^{(i,j)}$, $S_U^{(i,j)}$ spanning this space are indexed by i, j for which $i_{k_1} =$

$j_{k_1} = v_1$, ..., $i_{k_q} = j_{k_q} = v$, ..., $i_{k_p} = j_{k_p} = v_p$, and finally $i_l \neq j_l$ for $l \notin \{k_1, .., k_p\}$. Note that according to (48) the isomorphism Ψ maps these matrices into all matrices spanning $(\mathbb{M}_{U'})_{(k'_1,..,k'_{p-1}),(v_1,..,v_{q-1},v_{q+1},..,v_p)}$, where k'_1, ..., k'_{p-1} are defined in the lemma. This is because if we take any pair i, j designating $A_U^{(i,j)}$, $S_U^{(i,j)}$ spanning $(\mathbb{M}_U)_{(k_1,..,k_p),(v_1,..,v_p)}$, in the reduced vector index $[i_1, .., i_{k-1}, i_{k+1}, .., i_r]$ at positions k'_1, ..., k'_{p-1} we have subindices i_{k_1}, ..., $i_{k_{q-1}}$, $i_{k_{q+1}}$, ... i_{k_p} that are equal in pairs with subindices j_{k_1}, ..., $j_{k_{q-1}}$, $j_{k_{q+1}}$, ... j_{k_p} at the same positions in the vector index $[j_1, .., j_{k-1}, j_{k+1}, .., j_r]$. Their values are v_1, ..., v_{q-1}, v_{q+1}, ..., v_p, respectively. The only other pair of equal subindices, namely $i_{k_q} = j_{k_q} = v$, is absent from the reduced vector indices corresponding to i', j'. At other positions we get any possible pair of different values as we take any pair i, j allowed here, that is indexing $A_U^{(i,j)}$, $S_U^{(i,j)}$ spanning $(\mathbb{M}_U)_{(k_1,..,k_p),(v_1,..,v_p)}$. ■

Our most important result in this section is the following

Theorem 2.6 *The algebraic sum of subspaces in (24) is a direct sum.*

Proof

We will prove the following statement equivalent to the above theorem.

> Let $X_{(),()} \in (\mathbb{M}_U)_{(),()}$, $X_{(k_1,..,k_p),(v_1,..,v_p)} \in (\mathbb{M}_U)_{(k_1,..,k_p),(v_1,..,v_p)}$ for all possible choices of $(k_1, .., k_p)$ and $(v_1, .., v_p)$ be matrices whose sum is equal to a zero matrix. Then all these matrices (we will call them X-matrices) are zero matrices.

The proof will be by induction with respect to r, the number of factors in Kronecker product (12).

If we have only one factor, $U = U^{(1)}$, then $(\mathbb{M}_U)_{(),()} = \mathbb{M}_U$ is a direct sum of one component, namely $(\mathbb{M}_U)_{(),()}$.

Assume now that the theorem is true for any $(r-1)$ factor Kronecker product (12). In particular that what we stated above as eguivalent to our theorem is true for such a product.

Let our X-matrices add up to a zero matrix and let one of the summands, $X_{(k_1,..,k_p),(v_1,..,v_p)}$ be nonzero. Let $-X_{(k_1,..,k_p),(v_1,..,v_p)}$ be simply denoted by X. Thus X is the sum of the remaining X-matrices. We also need to introduce $k'_1 < k'_2 < ... < k'_{r-p}$ such that $\{k_1, .., k_p\} \cup \{k'_1, .., k'_{r-p}\} = \{1, .., r\}$.

The remaining X-matrices, forming X in a sum, can be split into two groups:

- Into one group we put these belonging to subspaces $(\mathbb{M}_U)_{(l_1,..,l_q),(w_1,..,w_q)}$ such that $k'_1 \notin \{l_1, .., l_q\}$. (An X-matrix belonging to $(\mathbb{M}_U)_{(),()}$ is in this group, if $\{k_1, .., k_p\}$ is nonempty. The other situation we consider at the end of the proof.) Thanks to that choice we can apply Lemma 2.4 **b)** to all of them, as well as to their sum, which will be denoted by Y:

$$\sum_{c_{k'_1}=1}^{n_{k'_1}} [Y]_{b,\left[:,..,:,c_{k'_1},:,..,:\right]} \quad = \quad \mathbf{0} \qquad \text{for any } b\text{-th row} \quad . \tag{49}$$

- Into the second group we put all the X-matrices which belong to $(\mathbb{M}_U)_{(l_1,..,l_q),(w_1,..,w_q)}$ such that $k'_1 \in \{l_1,..,l_q\}$, that is $l_s = k'_1$ for some $s \in \{1,..,q\}$, and then $w_s = v \in \{1,..,n_{k'_1}\}$. The group can further be split into subgroups corresponding to different values of v. When we add all the matrices in the whole group to form their sum Z, the b-th rows of Z, where the corresponding $[b_1,..,b_r]$ satisfy $b_{k'_1} = v$, are sums of b-th rows of matrices belonging only to the subgroup associated with value v. Matrices from other subgroups have at these positions zero rows.

  We can apply Lemma 2.4 **a)** to each matrix in a subgroup, as well as to their sum Z_v:

$$[Z_v]_{b,\left[:,..,:,c_{k'_1},:,..,:\right]} \quad = \quad \left| \left[U^{(k'_1)} \right]_{v,c_{k'_1}} \right|^2 \cdot \sum_{d_{k'_1}=1}^{n_{k'_1}} [Z_v]_{b,\left[:,..,:,d_{k'_1},:,..,:\right]} \tag{50}$$

  Since, as we have just said, matrices forming Z_v in a sum are responsible for formation of only those b-th rows for which $b_{k'_1} = v$, we can write for the sum Z of all Z_v :

$$[Z]_{\left[b_1,..,b_{k'_1},..,b_r\right],\left[:,..,:,c_{k'_1},:,..,:\right]} \quad = \quad \left| \left[U^{(k'_1)} \right]_{b_{k'_1},c_{k'_1}} \right|^2 \cdot \sum_{d_{k'_1}=1}^{n_{k'_1}} [Z]_{\left[b_1,..,b_{k'_1},..,b_r\right],\left[:,..,:,d_{k'_1},:,..,:\right]} \tag{51}$$

At this moment recall that, using our symbols, $X = Y + Z$. Also note that if one had to, one would classify X as belonging to the first group since $X \in (\mathbb{M}_U)_{(k_1,..,k_p),(v_1,..,v_p)}$ and $k'_1 \notin \{k_1,..,k_p\}$. So X satisfies (49) with Y replaced by X and analogous property holds for Z through the linear combination $Z = X - Y$. The last statement implies that the sums on the left hand side of (51) are zero rows, which in effect gives $Z = \mathbf{0}$. Further, let us return to component Z_v of Z. As Z is a zero matrix and Z_v have nonzero rows in disjoint regions, all Z_v must be zero matrices.

Recall that Z_v are formed by X-matrices belonging to all possible $(\mathbb{M}_U)_{(l_1,..,l_q),(w_1,..,w_q)}$ being subspaces of the larger space $\left(\tilde{M}_U\right)_{k'_1,v}$ introduced in Lemma 2.5 and spanned by $A_U^{(i,j)}$, $S_U^{(i,j)}$ with $i_{k'_1} = j_{k'_1} = v$. Lemma 2.5 tell us that this larger space is isomorphic to $\mathbb{M}_{U'}$ where $U' = U^{(1)} \otimes U^{(k'_1-1)} \otimes U^{(k'_1+1)} \otimes U^{(r)}$. We denote this isomorphism by Ψ, that is $\Psi\left(\left(\tilde{M}_U\right)_{k'_1,v}\right) = \mathbb{M}_{U'}$. In accordance with Lemma 2.5 we choose isomorphism Ψ such that it maps any space $(\mathbb{M}_U)_{(l_1,..,l_q),(w_1,..,w_q)}$ under consideration onto space $(\mathbb{M}_{U'})_{\left(l'_1,..,l'_{q-1}\right),(w_1,..,w_{s-1},w_{s+1},..,w_q)}$ where, as above, $l_s = k'_1,\ w_s = v,\ s \in$

$\{1,..,q\}$, and where l'_1, ..., l'_{q-1} are positions of l_1 ..., l_{s-1}, l_{s+1}, ..., l_q in the sequence $(1,2,...,k'_1-1,k'_1+1,...,r)$. In particular, $(\mathbb{M}_U)_{(l_s),(w_s)} = (\mathbb{M}_U)_{\left(k'_1\right),(v)}$ is mapped onto $(\mathbb{M}_{U'})_{(),()}$.

The images under Ψ of X-matrices forming Z_v are contained in the above mentioned image spaces $(\mathbb{M}_{U'})_{\left(l'_1,..,l'_{q-1}\right),(w_1,..,w_{s-1},w_{s+1},..,w_q)}$, which in turn are contained in $\mathbb{M}_{U'}$. The images add up to a zero matrix since the very X-matrices forming Z_v add up to a zero matrix.

On the other hand, and this is our induction assumption, $\mathbb{M}_{U'}$ is a direct sum of $(\mathbb{M}_{U'})_{\left(l'_1,..,l'_{q-1}\right),(w_1,..,w_{s-1},w_{s+1},..,w_q)}$, for we have all possible parameterizing pairs of sequences coming from all possible pairs $(l_1,..,l_q)$, $(w_1,..,w_q)$ such that $l_s = k'_1$, $w_s = v$ for some $s \in \{1,..,q\}$.

(According to Def. 2.1, sequences $(l_1,..,l_q)$ as well as $(l'_1,..,l'_{q-1})$ are ordered. Let sequences $(l'_1,..,l'_{q-1})$ and $(w_1,..,w_{s-1},w_{s+1},..,w_q)$ be given, with entries in appropriate ranges. Here s is defined to be such that $l'_1 < \ldots < l'_{s-1} < k'_1$. Then for $(l_1,..,l_q) = (l'_1,\ldots,l'_{s-1},k'_1,l'_s+1,\ldots,l'_{q-1}+1)$ and $(w_1,\ldots,w_{s-1},v,w_{s+1},..,w_q)$ space $(\mathbb{M}_U)_{(l_1,..,l_q),(w_1,..,w_q)}$ is mapped onto $(\mathbb{M}_{U'})_{\left(l'_1,..,l'_{q-1}\right),(w_1,..,w_{s-1},w_{s+1},..,w_q)}$.)

Thus all the images of X-matrices forming Z_v are zero matrices and the same must hold for the very X matrices. As v is taken to be an arbitrary element from the set $\{1,..,n_{k'_1}\}$, all matrices forming Z, that is belonging to the second group, are zero matrices. So X is formed only by matrices from the first group.

Analogous reasoning can be repeated with k'_2, ..., k'_{r-p} instead of k'_1. As a result we obtain that X is formed only by X-matrices belonging to $(\mathbb{M}_U)_{(l_1,..,l_q),(w_1,..,w_q)}$ such that k'_1, ..., k'_{r-p} do not belong to $\{l_1,..,l_q\}$ or, in other words, by X-matrices belonging to $(\mathbb{M}_U)_{\left(k_{g_1},..,k_{g_t}\right),(w_1,..,w_t)}$, where $\{k_{g_1},..,k_{g_t}\} \subset \{k_1,..,k_p\}$.

If one of these , call it X', is nonzero and belongs to $(\mathbb{M}_U)_{\left(k_{g_1},..,k_{g_t}\right),(w_1,..,w_t)}$ with $t < p$, that is $\{k_{g_1},..,k_{g_t}\} \neq \{k_1,..,k_p\}$, it can be expressed with the use of the remaining ones and X. We can repeat the whole reasoning with X' playing the role of X and k'_1 being replaced by some $k' \in \{1,..,r\} \setminus \{k_{g_1},..,k_{g_t}\}$ and simultaneously $k' \in \{k_1,..,k_p\}$. We then classify summand X as belonging to the second group of matrices, since $X \in (\mathbb{M}_U)_{(k_1,..,k_p),(v_1,..,v_p)}$ and $k' \in \{k_1,..,k_p\}$. We show as above that this second group of matrices consists of zero matrices which contradicts our assumption that $X \neq \mathbf{0}$.

Note that at this stage $(\mathbb{M}_U)_{(),()}$ could appear as $(\mathbb{M}_U)_{\left(k_{g_1},..,k_{g_t}\right),(w_1,..,w_t)}$. The short version of our reasoning for X (the role of X' at this stage) belonging to $(\mathbb{M}_U)_{(),()}$ is provided at the end of the proof. Also, precise repetition of our reasoning is always possible because no components in matrix sums are missing – even if we write that a matrix is formed only by some other matrices this means that the remaining ones are there as zero matrices.

Having $X \in (\mathbb{M}_U)_{(k_1,..,k_p),(v_1,..,v_p)}$ on the left, on the right we can only have nonzero components belonging to $(\mathbb{M}_U)_{(k_1,..,k_p),(w_1,..,w_p)}$ with $(w_1,..,w_p) \neq (v_1,..,v_p)$. Obviously $(w_1,..,w_p)$ are also distinct, since any component $(\mathbb{M}_U)_{(k_1,..,k_p),(w_1,..,w_p)}$ in what we aim to prove to be a direct sum, occurs only once. Collecting both sides together we get that the sum of X-matrices ($-X$ is one of them) belonging to $(\mathbb{M}_U)_{(k_1,..,k_p),(w_1,..,w_p)}$, for sequence $(k_1,..,k_p)$ fixed by the choice of X and for all possible sequences of values $(w_1,..,w_p)$, is a zero matrix. Since regions where these last candidates for nonzero X-matrices have nonzero rows do not overlap, also they must be zero matrices. This is exactly what we wanted to prove, hence indeed (24) is indeed the direct sum.

Now, as promised twice in this proof, we consider the case of $X \in (\mathbb{M}_U)_{(),()}$, that is the case of $\{k_1,..k_p\}$ being empty. Splitting the remaining summands into two groups, as previously, for any $k' \in \{k'_1,..,k'_r\} = \{1,..,r\}$, we conclude that any X-matrix belonging to $(\mathbb{M}_U)_{(l_1,..,l_q),(w_1,..,w_q)}$ such that $k' \in \{l_1,..,l_q\}$ is a zero matrix. Taking all k' under consideration we find that all X-matrices forming X must be zero matrices. So X must be a zero matrix too.

■

Let us rewrite (24) in a direct sum fashion:

$$\begin{aligned} \mathbb{M}_U \;=\; & \\ & (\mathbb{M}_U)_{(),()} \;\oplus\; \bigoplus_{k\in\{1..r\}} \bigoplus_{v\in\{1..n_k\}} (\mathbb{M}_U)_{(k),(v)} \;\oplus \\ & \oplus\; \bigoplus_{k_1<k_2\in\{1..r\}} \bigoplus_{(v_1,v_2)\in\{1..n_{k_1}\}\times\{1..n_{k_2}\}} (\mathbb{M}_U)_{(k_1,k_2),(v_1,v_2)} \;\oplus\; \dots \\ & \dots \;\oplus\; \bigoplus_{k_1<..<k_{r-1}\in\{1..r\}} \bigoplus_{(v_1,..,v_{r-1})\in\{1..n_{k_1}\}\times..\times\{1..n_{k_{r-1}}\}} (\mathbb{M}_U)_{(k_1,..,k_{r-1}),(v_1,..,v_{r-1})} \quad . \end{aligned} \tag{52}$$

Calculation of the defect of U requires calculation of the dimension of the $\mathbb{M}_U$, which luckily can be decomposed into the dimensions of the direct sum components. We will make this decomposition more informative in a moment.

3 Estimating the defect

Calculation of all the dimensions of the direct sum components in (52) can be reduced to calculation of dimensions of subspaces like $(\mathbb{M}_U)_{(),()}$ considered for subproducts of the Kronecker product U in (12).

Lemma 3.1 *There holds:*

$$\dim\Big((\mathbb{M}_U)_{(k_1,..,k_p),(v_1,..,v_p)}\Big) \;=\; \dim\Big((\mathbb{M}_{U^{\mathrm{p}}})_{(),()}\Big) \tag{53}$$

where

$$U^{\mathrm{p}} \;=\; \bigotimes_{k\in\{1..r\}\setminus\{k_1,..,k_p\}} U^{(k)} \tag{54}$$

is the original Kronecker product (12) deprived of its k_1-th, ..., k_p-th factors.

Proof
In the proof we use Lemma 2.5 repeatedly, assigning appropriate values to U, k and v. We have the following relations:

- Let $U = U$, the initial Kronecker product (12), and let $k = k_p$, $v = v_p$. Then by Lemma 2.5 $(\mathbb{M}_U)_{(k_1,..,k_p),(v_1,..,v_p)}$ is isomorphic to $(\mathbb{M}_{U'})_{(k_1,..,k_{p-1}),(v_1,..,v_{p-1})}$, where $U' = \bigotimes_{l\in\{1..r\}\setminus\{k_p\}} U^{(l)}$. In this case k'_1, ..., k'_{p-1} mentioned in Lemma 2.5 have values $k'_1 = k_1$, ..., $k'_{p-1} = k_{p-1}$, as they are the positions of k_1, ..., k_{p-1} in the sequence $(1, 2, ..., k_p - 1, k_p + 1, ..., r)$.

- Let $U = U'$, $k = k_{p-1}$ and $v = v_{p-1}$. Then $(\mathbb{M}_{U'})_{(k_1,..,k_{p-1}),(v_1,..,v_{p-1})}$ is isomorphic to $(\mathbb{M}_{U''})_{(k_1,..,k_{p-2}),(v_1,..,v_{p-2})}$, where $U'' = \bigotimes_{l\in\{1..r\}\setminus\{k_{p-1},k_p\}} U^{(l)}$.

- ...

- Let $U = U^{\mathrm{p}-1} = \bigotimes_{l\in\{1..r\}\setminus\{k_2..k_p\}} U^{(l)}$, and let $k = k_1$ and $v = v_1$. Then $(\mathbb{M}_{U^{\mathrm{p}-1}})_{(k_1),(v_1)}$ is isomorphic to $(\mathbb{M}_{U^{\mathrm{p}}})_{(),()}$, where $U^{\mathrm{p}} = \bigotimes_{l\in\{1..r\}\setminus\{k_1..k_p\}} U^{(l)}$.

Thus both subspaces mentioned in the lemma are isomorphic through the composition of the above listed isomorphisms, so they are of equal dimension. ■

Let us simplify our notation by introducing, for U being the product (12):

$$d^U_{\{k_1,..,k_p\}} \stackrel{\text{def}}{=} \dim\Big((\mathbb{M}_{U'})_{(),()}\Big) \quad \text{for} \quad U' = \bigotimes_{k\in\{1..r\}\setminus\{k_1..k_p\}} U^{(k)} \tag{55}$$

$$d^U_{\{\}} \stackrel{\text{def}}{=} \dim\Big((\mathbb{M}_U)_{(),()}\Big) \tag{56}$$

Using the fact that $\mathbb{M}_U$ is the direct sum (52) and that the dimension of any component space $(\mathbb{M}_U)_{(k_1,..,k_p),(v_1,..,v_p)}$ can be calculated by Lemma 3.1 to be $d^U_{\{k_1,..,k_p\}}$, the dimension of $\mathbb{M}_U$ can be expressed as in the Theorem 3.2 below.

At this point note also, that for a $(r-1)$-element set $\{k_1, ..., k_{r-1}\} = \{1..r\} \setminus \{s\}$ there holds $d^U_{\{k_1,..,k_{r-1}\}} = \dim\Big((\mathbb{M}_{U^{(s)}})_{(),()}\Big) = \dim(\mathbb{M}_{U^{(s)}})$. We do not assume any Kronecker product structure for $U^{(s)}$, that is vector indices are identical with ordinary indices here. Using such vector indices we cannot fix their only component, $(\mathcal{M}_{U^{(s)}})_{(1),(v)}$ would be empty.

Theorem 3.2 *Let U be a Kronecker product of unitary matrices (12). Then the dimension of the space $\mathbb{M}_U$ constructed for U according to (9) reads:*

$$\begin{aligned} \dim(\mathbb{M}_U) \quad = & \\ d^U_{\{\}} \;+\; \textstyle\sum_{k_1\in\{1..r\}} n_{k_1} \cdot d^U_{\{k_1\}} \;+\; \textstyle\sum_{k_1<k_2\in\{1..r\}} n_{k_1} n_{k_2} \cdot d^U_{\{k_1,k_2\}} \;+ \dots \\ + \textstyle\sum_{k_1<\ldots<k_{r-1}\in\{1..r\}} n_{k_1} \ldots n_{k_{r-1}} \cdot d^U_{\{k_1,..,k_{r-1}\}} \end{aligned} \tag{57}$$

Accordingly (see Definition 1.1), the defect of U equals to $(N-1)^2 - \dim(\mathbb{M}_U)$.

Maybe it is a good moment to wonder about applicability of our formulas when there are 1×1 Kronecker factors in product (12) forming U. This has been promised in the paragraph preceding Definition 2.1.

First, recalling this definition, consider subset $(\mathcal{M}_U)_{(k_1,k_2,..,k_p),(v_1,v_2,..,v_p)}$ of set $\mathcal{M}_U$. If $k \in \{1,..,r\} \setminus \{k_1,..,k_p\}$ and $n_k = 1$, this subset is empty. The reason is that you cannot find any $A_U^{(i,j)}$, $S_U^{(i,j)}$ belonging to it, that is indexed by i, j satisfying $i_k \neq j_k$, because $i_k, j_k \in \{1,..,n_k\} = \{1\}$. In this case let the corresponding subspace $(\mathbb{M}_U)_{(k_1,k_2,..,k_p),(v_1,v_2,..,v_p)}$ of space $\mathbb{M}_U$ be defined as the zero space $\{\mathbf{0}\}$, which is a space of dimension 0. In particular, when there are 1×1 factors in product (12), $(\mathcal{M}_U)_{(),()}$ is empty and $(\mathbb{M}_U)_{(),()}$ we define as the zero space. Consequently, $d^U_{\{k_1,..,k_p\}}$ has value 0, if for some $k \in \{1,..,r\} \setminus \{k_1,..,k_p\}$ there holds $n_k = 1$. In other words U', used in the definition (55) of $d^U_{\{k_1,..,k_p\}}$, must not contain any 1×1 Kronecker factors, if this $d^U_{\{k_1,..,k_p\}}$ is to be considered as a potentially nonzero number. (It still can be zero if for example U' is a permutation matrix, in which case all $A_{U'}^{(i,j)}$, $S_{U'}^{(i,j)}$ are zero matrices, so $(\mathbb{M}_{U'})_{(),()}$ is the zero space.)

Now, let us remove in sum (57) all components $d^U_{\{k_1,..,k_p\}}$ that must be zero due to the presence of 1×1 factors. What is left are only those $d^U_{\{k_1,..,k_p\}}$, for which there are no 1's left in sequence $(n_1,..,n_r)$ after removing the k_1-th, ..., k_p-th entries. The sum (57) truncated in this way looks as if it were written for U deprived of its 1×1 Kronecker factors, in which case we accept the validity of formula (57). This new U differs from the original one by a unimodular factor, so the space $\mathbb{M}_U$ and the defect $\mathbf{d}(U)$ remain the same, as one easily finds noting that first of all $A_U^{(i,j)}$, $S_U^{(i,j)}$ do not change with multiplication of U by a unimodular number. The answer to our question is thus: yes, we can use (57) in presence of 1×1 factors, provided that appropriate $d^U_{\{k_1,..,k_p\}}$ are assigned 0's.

This has some practical importance. For example, if we wanted to calculate defects for a large number of Kronecker products of at most r factors, we could store the sequences of sizes as rows of a matrix with r columns, filling rows with a certain number of 1's where the number of factors would be less than r. These rows would then be the input data for a procedure calculating the defect of an r factor Kronecker product of unitaries.

We can go even furher. Let us also, in this context, return to the direct sum formula (52). We have adopted above a convention, according to which $(\mathbb{M}_U)_{(k_1,k_2,..,k_p),(v_1,v_2,..,v_p)}$ is the zero space if there are 1's in sequence $(n_1,..,n_r)$ after removing from it the k_1-th, ..., k_p-th entries. Let us throw out these zero spaces from (52). We are left with $(\mathbb{M}_U)_{(k_1,k_2,..,k_p),(v_1,v_2,..,v_p)}$ where all k associated with $n_k = 1$ sit in $\{k_1,..,k_p\}$. But every such $(\mathbb{M}_U)_{(k_1,k_2,..,k_p),(v_1,v_2,..,v_p)}$ can be replaced by an equal space $(\mathbb{M}_{U'})_{\left(k'_1,k'_2,..,k'_{p'}\right),\left(v'_1,v'_2,..,v'_{p'}\right)}$, where:

- U' is U deprived of its 1×1 Kronecker factors, with the order of the remaining factors preserved,
- $(k'_1, k'_2, .., k'_{p'})$ contains the positions, of subsequent entries of the subsequence obtained from $(k_1,..,k_p)$ by throwing out all k's such that $n_k = 1$, in the subsequence

obtained from $(1,2,..,r)$ in the same way (This is cumbersome, being a consequence of our notation, and we met such formulation in Lemma 2.5.),

- $(v'_1, v'_2, .., v'_{p'})$ is the result of throwing out the entries (of the only possible value 1) out of $(v_1, v_2, .., v_p)$ corresponding to entries k of $(k_1, .., k_p)$ for which $n_k = 1$.

(Both spaces are equal because they are spanned by the same matrices. In general, $A_U^{(i,j)} = A_{U'}^{(i',j')}$, where i', j' correspond to the reduced vector indices obtained from the vector indices corresponding to i, j, respectively, by removing those k'th entries of these vector indices (entries necessarily equal to 1), for which k satisfies $n_k = 1$.)

After this truncation and replacement (52) looks as if it were written for U', in which case we accept the validity of the direct sum formula because U' does not contain 1×1 Kronecker factors. Since $\mathbb{M}_U = \mathbb{M}_{U'}$, the only difference between U and U' being a unimodular factor, the starting point direct sum with all those zero spaces appears to lead to the correct direct sum we would write if we first removed the 1×1 Kronecker factors. So, we can go either way, removing or leaving these factors.

It is interesting to give the lower bound for the defect of U being a Kronecker product, because, as it was pointed in the Introduction, for most unitaries the defect is zero. The lower bound we give here is associated with upper bounds on the dimensions $d^U_{\{k_1,..,k_p\}}$ of $(\mathbb{M}_{U'})_{(),()}$ for the Kronecker subproducts U' as defined in (55), all of which are in fact bounds on $d^U_{\{\}}$ with U replaced by an appropriate U'. All we need to know about these bounds is contained in the next lemma. Note that although we assume that the sizes of Kronecker factors are greater than 1, any factor of size 1 – a unimodular number – can be absorbed into one of the factors of size greater than 1.

Lemma 3.3 *Let U of size $N \times N$ be the Kronecker product (12) with $r \geq 1$ and factors $U^{(1)}$, ..., $U^{(r)}$ of size $n_1 \times n_1$, ..., $n_r \times n_r$, where all $n_k > 1$.*

Then the dimension of the space $(\mathbb{M}_U)_{(),()}$ constructed for U (Definition 2.2) is bounded in one of the following ways:

- *If $n_k > 2$ for any $k \in \{1..r\}$, then*
$$d^U_{\{\}} \quad \leq \quad (N-1)(n_1 - 1) \cdot \ldots \cdot (n_r - 1) \quad . \tag{58}$$

- *If $n_{k_1} = \ldots = n_{k_p} = 2$ for some distinct values $k_s \in \{1..r\}$, and for $k \notin \{k_1..k_p\}$ there holds $n_k > 2$, then*
$$d^U_{\{\}} \quad \leq \quad (N - 2^{p-1})(n_1 - 1) \cdot \ldots \cdot (n_r - 1) \quad . \tag{59}$$

Proof
From Lemma 2.4 **b)**, if $B \in (\mathbb{M}_U)_{(),()}$ the subrows of any of its rows satisfy, for any $k \in \{1..r\}$ (where c_k is at k-th position):
$$\sum_{c_k=1}^{n_k} [B]_{b,[:,..,:,c_k,:,..,:]} \quad = \quad \mathbf{0} \quad , \tag{60}$$

as in this case the role of the set $\{k_1, ..., k_p\}$ from Lemma 2.4 is played by an empty set. We will show that the b-th row of B can be parametrized by at most $(n_1-1)\cdot\ldots\cdot(n_r-1)$ independent parameters. For example, let $[B]_{b,[c_1,...,c_r]}$ be known for $c_1 \in \{1, .., (n_1-1)\}$, ..., $c_r \in \{1, .., (n_r-1)\}$. (60) determines the remaining entries in the following order:

- $[B]_{b,[n_1,c_2,..,c_r]} = -\sum_{c_1=1}^{(n_1-1)} [B]_{b,[c_1,c_2,..,c_r]}$ to make all $[B]_{b,[c_1,..,c_r]}$ known for $c_1 \in \{1, .., n_1\}$, $c_2 \in \{1, .., (n_2-1)\}$, ..., $c_r \in \{1, .., (n_r-1)\}$.
- $[B]_{b,[c_1,n_2,c_3,..,c_r]} = -\sum_{c_2=1}^{(n_2-1)} [B]_{b,[c_1,c_2,..,c_r]}$ to make all $[B]_{b,[c_1,..,c_r]}$ known for $c_1 \in \{1, .., n_1\}$, $c_2 \in \{1, .., n_2\}$ $c_3 \in \{1, .., (n_3-1)\}$, ..., $c_r \in \{1, .., (n_r-1)\}$.
- ...
- $[B]_{b,[c_1,c_2,c_3,..,c_{r-1},n_r]} = -\sum_{c_r=1}^{(n_r-1)} [B]_{b,[c_1,c_2,..,c_{r-1},c_r]}$ to have all the entries of $[B]_{b,:}$ known.

Next we show that the b-th row of B filled using the above algorithm, starting from those initially known $(n_1-1)\cdot\ldots\cdot(n_r-1)$ entries, satisfies (60) for any $k \in \{1..r\}$. That is, that the following equality holds for any $k \in \{1..r\}$ and $c_s \in \{1..n_s\}$ for any $s \in \{1..r\} \setminus \{k\}$:

$$[B]_{b,[c_1,..,c_{k-1},n_k,c_{k+1},..,c_r]} = -\sum_{d_k=1}^{n_k-1} [B]_{b,[c_1,..,c_{k-1},d_k,c_{k+1},..,c_r]} \quad . \tag{61}$$

Let in the above expression $c_{k_1} = n_{k_1}$, ..., $c_{k_p} = n_{k_p}$ and $c_s \neq n_s$ for $s \in \{1..r\} \setminus \{k_1, .., k_p\}$ with $k_1 < k_2 < \ldots < k_p$. By this we mean that $n_k = c_k = c_{k_q} = n_{k_q}$ for some $q \in \{1..p\}$. (Do not mistake k_1, ..., k_p for those from the second item of the lemma.) Then the left hand side of (61), where some of the entries are obtained using the algorithm from the dotted list above, reads:

$$\begin{aligned}
[B]_{b,[c_1,..,c_r]} &= \\
&-\sum_{d_{k_p}=1}^{(n_{k_p}-1)} [B]_{b,\left[c_1,..,d_{k_p},..,c_r\right]} = -\sum_{d_{k_p}=1}^{(n_{k_p}-1)} \left(-\sum_{d_{k_{p-1}}=1}^{(n_{k_{p-1}}-1)} [B]_{b,\left[c_1,..,d_{k_{p-1}},..,d_{k_p},..,c_r\right]}\right) = \ldots \\
&-\sum_{d_{k_p}=1}^{(n_{k_p}-1)} \left(-\sum_{d_{k_{p-1}}=1}^{(n_{k_{p-1}}-1)} \left(\ldots \left(-\sum_{d_{k_2}=1}^{(n_{k_2}-1)} \left(-\sum_{d_{k_1}=1}^{(n_{k_1}-1)} [B]_{b,\left[c_1,..,d_{k_1},..,d_{k_p},..,c_r\right]}\right)\right)\ldots\right)\right) = \\
-\sum_{d_{k_q}=1}^{(n_{k_q}-1)} &\left(-\sum_{d_{k_p}=1}^{(n_{k_p}-1)} \left(.. \left(-\sum_{d_{k_{q+1}}=1}^{(n_{k_{q+1}}-1)} \left(-\sum_{d_{k_{q-1}}=1}^{(n_{k_{q-1}}-1)} \left(.. \left(-\sum_{d_{k_1}=1}^{(n_{k_1}-1)} [B]_{b,\left[c_1,..,d_{k_1},..,d_{k_p},..,c_r\right]}\right)..\right)\right)\right)..\right)\right) \\
&= -\sum_{d_{k_q}=1}^{n_{k_q}-1} [B]_{b,\left[c_1,..,n_{k_1},..,n_{k_{q-1}},..,d_{k_q},..,n_{k_{q+1}},..,n_{k_p},..,c_r\right]} \\
&= -\sum_{d_{k_q}=1}^{n_{k_q}-1} [B]_{b,\left[c_1,..,c_{k_1},..,c_{k_{q-1}},..,d_{k_q},..,c_{k_{q+1}},..,c_{k_p},..,c_r\right]} \\
&= -\sum_{d_k=1}^{n_k-1} [B]_{b,[c_1,..,d_k,..,c_r]} \quad ,
\end{aligned} \tag{62}$$

and equals thus to the right hand side of (61)

In this way each row of $B \in (\mathbb{M}_U)_{(),()}$ could be potentially parametrized by no more than $(n_1-1)\cdot\ldots\cdot(n_r-1)$ parameters – if there were no other restrictions caused by the structure of $U^{(s)}$ – but we need to parameterize only $N-1$ rows in general. This is caused by the property that all column sums in B are zeros, just as is the case with the spanning matrices $A_U^{(i,j)}$, $S_U^{(i,j)}$. Hence, in general, we have no more than $(N-1)\cdot(n_1-1)\cdot\ldots\cdot(n_r-1)$ free parameters to determine B. In other words: all $B \in (\mathbb{M}_U)_{(),()}$ belong to a single space of dimension $(N-1)(n_1-1)\cdot\ldots\cdot(n_r-1)$.

The case when some n_k are equal to 2 is a separate one, but what really counts is when there are more than one n_k equal to 2.

In this case let again $B \in (\mathbb{M}_U)_{(),()}$ and let $n_{k_1} = 2$, ..., $n_{k_p} = 2$. The $[b_1,..,b_r]$-th row of B is a linear combination of $[b_1,..,b_r]$-th rows of $A_U^{(i,j)}$, $S_U^{(i,j)}$ such that, among other conditions, $i_{k_1} = 2/j_{k_1}$, ..., $i_{k_p} = 2/j_{k_p}$, where of course $i_{k_q}, j_{k_q} \in \{1,2\}$.

Consider the group of rows in B indexed by such $[b_1,..,b_r]$ that for some chosen values $s_1,...,s_p \in \{1,2\}$ the vector index satisfies

$$\big(b_{k_1} = s_1\ ,\ \ldots\ ,\ b_{k_p} = s_p\big) \quad \text{or} \quad \big(b_{k_1} = 2/s_1\ ,\ \ldots\ ,\ b_{k_p} = 2/s_p\big)\ . \tag{63}$$

Observe now that the rows of B from this group are linear combinations of respective nonzero rows of only those $A_U^{(i,j)}$, $S_U^{(i,j)}$ (from the collection of those spanning $(\mathbb{M}_U)_{(),()}$) which are indexed by i, j satisfying:

$$\big[i_{k_1},..,i_{k_p}\big]\,,\ \big[j_{k_1},..,j_{k_p}\big] \quad \in \quad \{\ [s_1,..,s_p]\,,\ [2/s_1,..,2/s_p]\ \}\ . \tag{64}$$

Since subsets of (i,j)'s (of the set of all (i,j)'s indexing $A_U^{(i,j)}$, $S_U^{(i,j)}$ spanning $(\mathbb{M}_U)_{(),()}$) fulfilling condition (64) for fixed $s_1,...,s_p$ are disjoint, also disjoint are the subsets of $(\mathcal{M}_U)_{(),()}$ of those corresponding $A_U^{(i,j)}$, $S_U^{(i,j)}$ which are nonzero matrices. Within each such subset, associated with (64), the nonzero rows of its members hit the index area defined in (63). Therefore the matrices $A_U^{(i,j)}$, $S_U^{(i,j)}$ belonging to it not only have the property that their rows add up to a zero row, but also that all the rows of such a matrix indexed by $[b_1,..,b_r]$ satisfying (63) add up to a zero row.

Thus, through a linear combination, in the considered group of rows in B one of the rows depends on others. We have $2^p/2 = 2^{p-1}$ possible choices of $[s_1,..,s_p]$, hence 2^{p-1} groups (of the specified type) of rows in B with 2^{p-1} dependent rows altogether. Using the previous method of parameterizing rows, we can parameterize no more than $(N-2^{p-1})$ rows, introducing no more than $(n_1-1)\cdot\ldots\cdot(n_r-1)$ parameters into each row. In other words: B being contained in the described above $(N-2^{p-1})(n_1-1)\cdot\ldots\cdot(n_r-1)$ dimensional space is a necessary condition for B being a member of $(\mathbb{M}_U)_{(),()}$.

Our final remark will concern the case when we deal with a one factor Kronecker product, $r = 1$, $U = U^{(1)}$, $N = n_1$. The bound, either formula (58) or formula (59), takes then the form $(N-1)^2$. This agrees with these facts:

- $\dim((\mathbb{M}_U)_{(),()}) \ = \ \dim(\mathbb{M}_U)$, no Kronecker product structure assumed for U.
- $\mathbb{M}_U$ is contained in the space tangent to the set of all $N \times N$ doubly stochastic matrices, that is the space of all real $N \times N$ matrices in which entries in any row or column add up to 1. This space is of dimension $(N-1)^2$.

■

In what follows Theorem 3.2 there are arguments behind defining $(\mathbb{M}_U)_{(),()}$ as the zero space if there are 1×1 Kronecker factors in (12) not absorbed into larger factors, and that $d^U_{\{\}}$ has to be assigned 0 then. In this case we can also use the bound (58) or (59) which produces the correct dimension 0.

Having the above result of Lemma 3.3 let us replace the values $d^U_{\{k_1,..,k_p\}}$ in Theorem 3.2 by their upper bounds being the appropriate right hand sides of (58) and (59). We will get an upper bound on $\dim(\mathbb{M}_U)$, equivalently a lower bound on the defect $\mathbf{d}(U) = (N-1)^2 - \dim(\mathbb{M}_U)$.

What is more, this can be done successfully also in the presence of unabsorbed 1×1 Kronecker factors. Since the bounds (58), (59) yield 0 for $d^U_{\{k_1,..,k_p\}}$ corresponding to zero spaces in the direct sum (52), whose presence is associated with the 1×1 factors, bounding the dimensions of these spaces does not affect the total upper bound on $\dim(\mathbb{M}_U)$ at all, that is we obtain the value we would get if the 1×1 factors were first absorbed into larger factors. This can be better understood if one carefully follows the reasoning following Theorem 3.2. The practical consequence is this: if one had some other bounds on $d^U_{\{k_1,..,k_p\}}$, yielding zeros for spaces that are necessarily zero spaces because of 1×1 factors, one could leave the 1×1 factors unabsorbed.

To better expose properties of our bound, it is convenient to introduce another notion, the *generalized defect* $\mathbf{D}(U)$ of a unitary U, defined as

$$\mathbf{D}(U) \quad = \quad \mathbf{d}(U) + (2N-1) \quad = N^2 - \dim(\mathbb{M}_U) \quad = \dim\left((\mathbb{M}_U)^{\perp}\right) \tag{65}$$

When we recall expressions in (8) and the preceding formulas it will be clear that $\mathbf{D}(U)$ is the dimension of the space (1), that is the space:

$$\mathbb{V}_U \quad = \quad \{R \ : \ \mathbf{i}R \circ U \ = \ EU \quad \text{for some antihermitian } E\} \tag{66}$$

We use in our new definition the word *generalized* because the definition of $\mathbf{d}(U)$ is suited for the class of unitary matrices which have the dimension of manifold $\{D_r \cdot U \cdot D_c \ : \ D_r, D_c \text{ unitary diagonal}\}$ equal to $2N-1$. Because of some applications of the defect mentioned in the Introduction it is more convenient subtract the dimension of this manifold from $\mathbf{D}(U)$ to define the defect associated with other type of U.

The corresponding lower bound on $\mathbf{D}(U)$ will be, thanks to Theorem 3.2 and Lemma 3.3 and definitions (55), (56). :

$$
\begin{aligned}
&(n_1 \cdot \ldots \cdot n_r)^2 \quad - \\
&- \Bigg(\Bigg(\prod_{l\in\{1..r\}} n_l \; - \; 2^{(\sharp_2\{1..r\})-1} \Bigg) \cdot \prod_{l\in\{1..r\}} (n_l - 1) \quad + \\
&\sum_{k_1\in\{1..r\}} \Bigg(n_{k_1} \Bigg(\prod_{l\in\{1..r\}\setminus\{k_1\}} n_l \; - \; 2^{(\sharp_2\{1..r\}\setminus\{k_1\})-1} \Bigg) \cdot \prod_{l\in\{1..r\}\setminus\{k_1\}} (n_l - 1) \Bigg) \quad + \\
&\sum_{k_1<k_2\in\{1..r\}} \Bigg(n_{k_1} n_{k_2} \Bigg(\prod_{l\in\{1..r\}\setminus\{k_1,k_2\}} n_l \; - \; 2^{(\sharp_2\{1..r\}\setminus\{k_1,k_2\})-1} \Bigg) \cdot \prod_{l\in\{1..r\}\setminus\{k_1,k_2\}} (n_l - 1) \Bigg) \quad + \quad \ldots \quad + \\
&\sum_{k_1<\ldots<k_{r-1}\in\{1..r\}} \Bigg(n_{k_1} \ldots n_{k_{r-1}} \Bigg(\prod_{l\in\{1..r\}\setminus\{k_1..k_{r-1}\}} n_l \; - \; 2^{(\sharp_2\{1..r\}\setminus\{k_1..k_{r-1}\})-1} \Bigg) \cdot \prod_{l\in\{1..r\}\setminus\{k_1..k_{r-1}\}} (n_l - 1) \Bigg) \Bigg) \quad ,(67)
\end{aligned}
$$

where for a nonempty subset $\mathcal{A} = \{l_1, ..., l_s\}$ of $\{1, ..., r\}$ expression $\sharp_2\mathcal{A}$ denotes

- the number of 2's in sequence $(n_{l_1}, ..., n_{l_s})$, if there are any,
- 1 otherwise.

Although the above expression looks very complicated, below we show that it is, almost, a mere product of trivial functions of the sizes n_1, ..., n_r of factors of the considered Kronecker product.

Because in Lemma 3.3 it was assumed that all Kronecker factors are of size greater than 1, formally (67) is a valid lower bound only in this situation, therefore we confine ourselves in the formulation of the theorem below. But, in the paragraph preceding the one containing the definition (65) of the generalized defect, we argued that even in the presence of 1×1 Kronecker factors the total bound (67), obtained by substituting (58, 59) into (57), will be equal to the value (67) obtained for the Kronecker product with absorbed 1×1 factors (this can be also guessed purely by analyzing (67) as a function of sequence of sizes $(n_1, .., n_r)$). Let us leave it as a comment that (67) must, in the presence of 1×1 factors, lead to (68) or (69) deprived of its factors $(2n_l - 1)$ corresponding to $n_l = 1$, but since then $2n_l - 1 \; = \; 1$, in Theorem 3.4 one does not need to assume that all $n_k > 1$.

Theorem 3.4 *The lower bound (67) on the generalized defect (definition (65)) of U being the Kronecker product (12) with factors $U^{(1)}$, ..., $U^{(r)}$ of size $n_1 \times n_1$, ..., $n_r \times n_r$ respectively, where all $n_k > 1$, is equal to*

a)

$$\prod_{l\in\{1..r\}} (2\cdot n_l \;-\; 1)\,, \tag{68}$$

if all $n_k > 2$*,*

b)

$$\left(\prod_{l\in\{1..r\},\ n_l>2} (2\cdot n_l \;-\; 1)\right)\cdot 2^{(\sharp_2\{1..r\})-1}\left(2^{(\sharp_2\{1..r\})} \;+\; 1\right)\quad , \tag{69}$$

if there is at least one 2 *in the sequence* $(n_1,...,n_r)$*, where* $\sharp_2\{1..r\}$ *is the number of* 2*'s in this sequence.*

Proof
We need to show that there holds an equality between two values, one being a relatively simple polynomial expression:

a)

$$\left(\prod_{l\in\{1..r\}} n_l\right)\cdot\left(\prod_{l\in\{1..r\}} ((n_l-1)\;+\;1)\right) \;-\; \prod_{l\in\{1..r\}} (n_l\;+(n_l-1)) \tag{70}$$

if all $n_k > 2$,

b)

$$\left(\prod_{l\in\{1..r\}} n_l\right)\cdot\left(\prod_{l\in\{1..r\}} ((n_l-1)\;+\;1)\right) - \left(\prod_{l\in\{1..r\},\ n_l>2} (n_l\;+(n_l-1))\right)\cdot 2^{(\sharp_2\{1..r\})-1}\left(2^{(\sharp_2\{1..r\})}\;+\;1\right), \tag{71}$$

if $n_k = 2$ for some $k\in\{1,...,r\}$.

and the other being the long expression in the most outer bracket in (67). This last expression will be simply referred to as (67)'. We will compare the above mentioned two quantities component by component.

We start from the p-th component of (67)', by which we mean:

$$\sum_{k_1<...<k_p\in\{1..r\}}\left(n_{k_1}...n_{k_p}\left(\prod_{l\in\{1..r\}\setminus\{k_1..k_p\}} n_l \;-\; 2^{(\sharp_2\{1..r\}\setminus\{k_1..k_p\})-1}\right)\cdot\prod_{l\in\{1..r\}\setminus\{k_1..k_p\}} (n_l-1)\right)\quad . \tag{72}$$

Step 1 The, call it, left part being the result of taking only the left product from the inner bracket in (72) is equal to:

$$\sum_{k_1<...<k_p\in\{1..r\}}\left(\prod_{l\in\{1..r\}} n_l\cdot\prod_{l\in\{1..r\}\setminus\{k_1..k_p\}} (n_l-1)\right)\quad . \tag{73}$$

The above sum can also be found in the expansion of the left product of (70) or (71). Any component of the above sum is the result of choosing, in the right subproduct of the left product of (70, 71), p brackets at positions k_1, ..., k_p from which 1's will be taken to be multiplied with $(n_l - 1)$'s from the remaining $r - p$ brackets. Thus every left part (73) for $p = 1..(r-1)$ has its counterpart in the left product of (70, 71).

On the other hand, in the expansion of this product there are two components, namely $(n_1 \cdot \ldots \cdot n_r)(n_1 - 1) \cdot \ldots \cdot (n_r - 1)$ and $(n_1 \cdot \ldots \cdot n_r)$ so far unexplained. We easily see that the first one is the left part of the 0-th component of (67)':

$$\left(\prod_{l \in \{1..r\}} n_l \; - \; 2^{(\sharp_2\{1..r\})-1} \right) \cdot \prod_{l \in \{1..r\}} (n_l - 1) \tag{74}$$

The second one still have to be found.

Step 2 The, call it, right part of (72) looks like this:

$$- \sum_{k_1 < \ldots < k_p \in \{1..r\}} \left(n_{k_1} \ldots n_{k_p} \cdot 2^{(\sharp_2\{1..r\} \setminus \{k_1..k_p\})-1} \cdot \prod_{l \in \{1..r\} \setminus \{k_1..k_p\}} (n_l - 1) \right) \quad . \tag{75}$$

The expression under the sum, given for some $k_1, ..., k_p$, can be further transformed into:

- $$\left(\prod_{\{q:\; n_{k_q} \neq 2\}} n_{k_q} \right) \cdot 2^{(\sharp_2\{1..r\})-1} \cdot \prod_{l \in \{1..r\} \setminus \{k_1..k_p\},\; n_l \neq 2} (n_l - 1) \tag{76}$$

  if there are no 2's in $(n_1, ..., n_r)$ or if there are 2's in $(n_{l_1}, ..., n_{l_{r-p}})$ where $\{l_1, .., l_{r-p}\} = \{1, .., r\} \setminus \{k_1, .., k_p\}$.

- $$\left(\prod_{\{q:\; n_{k_q} \neq 2\}} n_{k_q} \right) \cdot 2^{(\sharp_2\{1..r\})-1} \cdot \left(\prod_{l \in \{1..r\} \setminus \{k_1..k_p\},\; n_l \neq 2} (n_l - 1) \right) \cdot 2 \tag{77}$$

  if there are no 2's in $(n_{l_1}, ..., n_{l_{r-p}})$ and there are some in $(n_{k_1}, .., n_{k_p})$, where $\{l_1, .., l_{r-p}\}$ is as above. Note that in this situation the additional 2 at the end is caused by the fact that $\sharp_2\{l_1, .., l_{r-p}\} = 1$ due to the definition of $\sharp_2$.

So, in the sum (75) we add expressions like (76) or (77) depending on how 2's are scattered among the considered subsequences of $(n_1, ..., n_r)$. And we do this over all $p = 1...(r-1)$ in the total sum in (67)'.

Next we will add only those summands in the sum of all right parts (75) over $p = 1...(r-1)$, which are associated with sequences $(k_1, ..., k_p)$ containing a given fixed subsequence $(k_{q_1}, ..., k_{q_t}) = (s_1, ..., s_t)$ such that n_{s_1}, ..., n_{s_t} are all greater than 2, and which (these $(k_1, .., k_p)$'s) are such that for any k_j not belonging to this subsequence $n_{k_j} = 2$. The sizes n_{s_1}, ..., n_{s_t} play the role n_{k_q} of (76) and (77). All sequences are assumed to be increasing ones.

- For $p = t$ we add nothing to build $(k_1, ..., k_p)$ out of $(k_{q_1}, ..., k_{q_t})$, therefore we have only one such summand, here $q_1 = 1, ..., q_t = p$. The number of summands is equal to $\binom{\sharp_2\{1..r\}}{0}$. Formula (76) is used for a summand.
- For $p = t + 1$, the number of summands is equal to 0 if there are no 2's in $(n_1, ..., n_r)$, or $\binom{\sharp_2\{1..r\}}{1}$, that is the number of ways in which we can extend $(k_{q_1}, ..., k_{q_t})$ to $(k_1, ..., k_p)$ by such k that $n_k = 2$. For a summand the formula (76) is used if there are at least two 2's in $(n_1, .., n_r)$, that is if there is at least one 2 outside $(n_{k_1}, ..., n_{k_p})$. Otherwise formula (77) is used for a summand.
- For $p = t+2$ the number of summands is 0 if there is only one 2 in $(n_1, ..., n_r)$, or $\binom{\sharp_2\{1..r\}}{2}$ if there are at least two. If there are more than two 2's in $(n_1, ..., n_r)$ formula (76) is used for a summand, otherwise we use (77)
- ...
- If $p = t + \sharp_2\{1..r\}$ and $p \leq r - 1$ the number of summands is either 0 or $\binom{\sharp_2\{1..r\}}{\sharp_2\{1..r\}}$. In this case there are no more 2's in $(n_1, ..., n_r)$ outside $(n_{k_1}, ..., n_{k_p})$, therefore we use formula (77) for this single summand. (This all applies if there are 2's in $(n_1, ..., n_r)$. If there are no 2's, we end with $p = t$.)
- If $p = r - 1$ and $\sharp_2\{1..r\} = r - t$, then $p = t + \sharp_2\{1..r\} - 1$, the number of summands is either zero or it is equal to $\binom{\sharp_2\{1..r\}}{\sharp_2\{1..r\}-1}$. Since there is one 2 left in $(n_1, ..., n_r)$ outside $(n_{k_1}, ..., n_{k_p})$ we use (76) for all summands considered here. (This again applies if there are 2's in $(n_1, ..., n_r)$.)

Having calculated the number of summands in each particular case, the sum of all of them, with sign $-$ inherited from (75):

$$-\sum_{p=1}^{r-1} \sum_{\substack{(k_1, ..., k_p) \text{ s.t.} \\ (k_{q_1}, .., k_{q_t}) = (s_1, ..., s_t) \\ \text{for some } q_1, .., q_t}} \left(n_{k_1} ... n_{k_p} \cdot 2^{(\sharp_2\{1..r\} \setminus \{k_1..k_p\})-1} \cdot \prod_{l \in \{1..r\} \setminus \{k_1..k_p\}} (n_l - 1) \right) \tag{78}$$

takes the following forms.

- If there are no 2's in the sequence $(n_1, .., n_r)$

$$-\left(\prod_{i=1}^{t} n_{s_i} \right) \cdot 2^{(\sharp_2\{1..r\})-1} \cdot \left(\prod_{l \in \{1..r\} \setminus \{s_1..s_t\},\ n_l \neq 2} (n_l - 1) \right) \cdot 1 \quad , \tag{79}$$

(78) equals to

$$-\left(\prod_{i=1}^{t} n_{s_i}\right) \cdot \prod_{l\in\{1..r\}\setminus\{s_1..s_t\}} (n_l - 1) \quad . \tag{80}$$

In fact, in this case it is better to analyze directly (75), where, by taking $p = 1, ..., r-1$, one finds that any summand has its counterpart in the right product of (70). Namely, (80) for $(s_1, ..., s_t) = (k_1, ..., k_p)$ is the result of choosing n_l from brackets at positions k_1, ..., k_p in the right product of (70), to be multiplied by $(n_l - 1)$ from the remaining brackets. The additional summands in an expansion of the right product of (70) are the product of all n_k's, $n_1 \cdot \ldots \cdot n_r$, which compensates for an identical product in an expansion of the left product of (70), we searched for this earlier at **Step 1**, and finally the product of all $(n_k - 1)$'s which in turn can be found in the 0'th component (74) of (67)', on the other side of the equality between (70) and (67)' being proved. Thus we are completely done with the case when there are no 2's in $(n_1, ..., n_r)$.

- If the are some 2's in the sequence $(n_1, ..., n_r)$:

Case 1 If $t + \sharp_2\{1, ..., r\} \leq r - 1$ then (78) equals to

$$-\left(\prod_{i=1}^{t} n_{s_i}\right) \cdot 2^{(\sharp_2\{1..r\})-1} \cdot \prod_{l\in\{1..r\}\setminus\{s_1..s_t\},\ n_l\neq 2} (n_l - 1) \cdot$$
$$\cdot \left(\binom{\sharp_2\{1..r\}}{0} + \binom{\sharp_2\{1..r\}}{1} + \binom{\sharp_2\{1..r\}}{2} + \ldots + \binom{\sharp_2\{1..r\}}{\sharp_2\{1..r\}} + 1\right) \quad ,(81)$$

In this case we can extend $(s_1, ..., s_t)$ to $(k_1, ..., k_p)$ in such a way that $(n_{k_1}, ..., n_{k_p})$ contains all 2's from $(n_1, ..., n_r)$. The summand associated with such $(k_1, ..., k_p)$ is expressed with the use of (77), in which we have an additional factor 2. That is why expression of type (76) standing in the top part of (81) has to be added twice, and hence the last 1 in the rightmost bracket of (81). This expression finally takes the form:

$$-\left(\prod_{i=1}^{t} n_{s_i}\right) \cdot 2^{(\sharp_2\{1..r\})-1} \cdot \left(\prod_{l\in\{1..r\}\setminus\{s_1..s_t\},\ n_l\neq 2} (n_l - 1)\right) \cdot \left(2^{(\sharp_2\{1..r\})} + 1\right) \quad . \tag{82}$$

Case 2 If $t + \sharp_2\{1, ..., r\} = r$, that is $t = r - \sharp_2\{1, ..., r\}$ we get for (78)

$$-\left(\prod_{i=1}^{t} n_{s_i}\right) \cdot 2^{(\sharp_2\{1..r\})-1} \cdot \prod_{l\in\{1..r\}\setminus\{s_1..s_t\},\ n_l\neq 2} (n_l - 1) \cdot$$
$$\cdot \left(\binom{\sharp_2\{1..r\}}{0} + \binom{\sharp_2\{1..r\}}{1} + \binom{\sharp_2\{1..r\}}{2} + \ldots + \binom{\sharp_2\{1..r\}}{\sharp_2\{1..r\}-1}\right) \quad ,(83)$$

In other words, outside the subsequence $(n_{s_1},...,n_{s_t})$ there are only 2's in the sequence $(n_1,...,n_r)$. Every summand associated with $(k_1,...,k_p)$ produced out of such $(s_1,...,s_t)$ is expressed with the use of (76). Note that in the case of only one 2 in $(n_1,...,n_r)$ the sum of binomials containes only $\binom{1}{0}$. The sum (83) takes the final form:

$$
\begin{aligned}
&-\left(\prod_{i=1}^{t} n_{s_i}\right)\cdot 2^{(\sharp_2\{1..r\})-1}\cdot\left(\prod_{l\in\{1..r\}\setminus\{s_1..s_t\},\ n_l\neq 2}(n_l-1)\right)\cdot\left(2^{(\sharp_2\{1..r\})}-1\right) \quad = \\
&-\left(\prod_{i=1}^{t} n_{s_i}\right)\cdot 2^{(\sharp_2\{1..r\})-1}\cdot\left(\prod_{l\in\{1..r\}\setminus\{s_1..s_t\},\ n_l\neq 2}(n_l-1)\right)\cdot\left(2^{(\sharp_2\{1..r\})}+1\right) \quad + \\
&\qquad\left(\prod_{i=1}^{t} n_{s_i}\right)\cdot 2^{(\sharp_2\{1..r\})}\cdot\left(\prod_{l\in\{1..r\}\setminus\{s_1..s_t\},\ n_l\neq 2}(n_l-1)\right)
\end{aligned} \tag{84}
$$

The reader should realize, that the **Case** 2 occures only once, when $(s_1,...,s_t)$ is of maximal length. Then we get an additional component, the second part of (84). In general we add expressions like (82), over all possible nonempty sequences $(s_1,...,s_t)$, that is over all t ranging from 1 to $r-(\sharp_2\{1..r\})$. So let us first concentrate on them.

As in the case without 2's in $(n_1,...,n_r)$ we note that any expression like (82) has its counterpart in the right product of (71). Again it is a matter of choosing brackets from which we take n_l's, at the positions corresponding to the positions of $s_1,...,s_t$ in the increasing subsequence $(k:\ n_k>2)$ of $(1,...,r)$. Note that in this process we also deal with the situation when all $n_k>2$ are used in (82), in fact in the 'standard' part of (84) ($(s_1,...,s_t)$ of maximum length, **Case 2** above), which corresponds to taking only n_l's from brackets in (71).

What remains in an expansion of (71) are the values:

$$
-\left(\prod_{l\in\{1..r\},\ n_l>2}(n_l-1)\right)\cdot 2^{(\sharp_2\{1..r\})-1}\left(2^{(\sharp_2\{1..r\})}\ +\ 1\right) \qquad \text{and} \tag{85}
$$

$$
\prod_{l\in\{1..r\}} n_l, \tag{86}
$$

where the last product was mentioned as unexplained at the end of **Step** 1.

On the other side, in (67)', we have still left the right part of the 0-th component (74) of (67)', which can be written as:

$$
-\left(\prod_{l\in\{1..r\},\ n_l>2}(n_l-1)\right)\cdot 2^{(\sharp_2\{1..r\})-1}\quad , \tag{87}
$$

the additional component in (84) occuring only for $(s_1, ..., s_t)$ of maximum length, therefore written as

$$\left(\prod_{\{l:\ n_l>2\}} n_l \right) \cdot 2^{(\sharp_2\{1..r\})} \quad , \tag{88}$$

and finally all summands in the left parts (75) for $p = 1, ..., r-1$ which are associated with sequences $(k_1, ..., k_p)$ such that there are only 2's in $(n_{k_1}, ..., n_{k_p})$. We add these summands in **Step 3** which completes the proof.

Step 3 The expression under the sum in (75), in case of $(k_1, ..., k_p)$ such that $(n_{k_1}, ..., n_{k_p}) = (2, ..., 2)$, takes the form

- $$2^{(\sharp_2\{1..r\})-1} \cdot \prod_{\{l:\ n_l>2\}} (n_l - 1) \tag{89}$$

  if the number of 2's in $(n_1, ..., n_r)$ is greater than p,

- $$2^{(\sharp_2\{1..r\})-1} \cdot \left(\prod_{\{l:\ n_l>2\}} (n_l - 1) \right) \cdot 2 \tag{90}$$

  if the number of 2's in $(n_1, ..., n_r)$ is equal to p, $p = (\sharp_2\{1..r\})$. This is again caused by the definition of $\sharp_2$. In this case $2^{(\sharp_2\{1..r\}\setminus\{k_1..k_p\})}$ is equal to 2 while there are no 2's among n_k indexed by $k \in \{1..r\} \setminus \{k_1..k_p\}$.

Now we calculate how many summands of this type can be found in the sum of all the right parts (75). It is assumed that at least one 2 can be found in $(n_1, ..., n_r)$. The other case has been completely resolved in the paragraph following formula (80).

- For $p = 1$ the number of summands is equal to $\binom{\sharp_2\{1..r\}}{1}$, the number of ways we choose a one element subsequence, containing only 2's, from $(n_1, ..., n_r)$. We use (90) for a summand if there is only one 2 in $(n_1, ..., n_r)$, otherwise we use (89).
- For $p = 2$ the number of summands is either 0 if there is only one 2 in $(n_1, ..., n_r)$, or $\binom{\sharp_2\{1..r\}}{2}$, we choose a two element subsequence this time. We use (90) for each summand if there are only two 2's in $(n_1, ..., n_r)$, or we use (89) if there are at least three.
- ...
- For $p = \sharp_2\{1..r\}$ the number of summands is $\binom{\sharp_2\{1..r\}}{\sharp_2\{1..r\}}$ and we of course use formula (90) for this single summand.

We add all the considered summands below, where the negative sign is inherited from (75). In the first sum we still use the form of a summand originating from (75):

$$-\sum_{p=1}^{r-1} \sum_{\substack{(k_1,...,k_p) \text{ s.t.} \\ (n_{k_1},...,n_{k_p})=(2,2,...,2)}} \left(n_{k_1}...n_{k_p} \cdot 2^{(\sharp_2\{1..r\}\setminus\{k_1..k_p\})-1} \cdot \prod_{l\in\{1..r\}\setminus\{k_1..k_p\}} (n_l-1) \right) =$$

$$-\ 2^{(\sharp_2\{1..r\})-1} \cdot \prod_{\{l:\ n_l>2\}} (n_l-1) \cdot \left(\binom{\sharp_2\{1..r\}}{1} + \binom{\sharp_2\{1..r\}}{2} + \ldots + \binom{\sharp_2\{1..r\}}{\sharp_2\{1..r\}} + 1 \right) \tag{91}$$

where the last 1 is the result of applying formula (90), with that additional multiplication by 2, to the single summand for $p = \sharp_2\{1..r\}$. The final result is thus:

$$-\left(\prod_{\{l:\ n_l>2\}} (n_l-1) \right) \cdot 2^{(\sharp_2\{1..r\})-1} \cdot 2^{(\sharp_2\{1..r\})} \tag{92}$$

This is the end. What is left for us to say is that:

- (92) together with (87), both within (67)', compensate for (85) being part of (71).
- (88), a part of (67)', is equal to (86) coming from (71).

■

Our calculation of the bound (68, 69) on the generalized defect $\mathbf{D}(U)$ of U given by (12) is based on the formula for the dimension of $\mathbb{M}_U$ given by Theorem 3.2, which in turn is based on the decomposition of $\mathbb{M}_U$ into direct sum components provided by Theorem 2.6. As far as the case with no 2's in the sequence of sizes $(n_1,...,n_r)$ is concerned, we can use a simpler reasoning leading to the corresponding bound (68). To this end let us consider the following lemma, in which we use spaces defined in (66).

Lemma 3.5 *Let U and V be unitary matrices of size $N\times N$ and $M\times M$ respectively. Let $R\in\mathbb{V}_U$ and $S\in\mathbb{V}_V$, where R,S are real matrices of the size identical with that of U,V, respectively.*

Then $R\otimes S \ \in\ \mathbb{V}_{U\otimes V}$.

Proof
From the assumptions there holds

$$\mathbf{i}R\circ U \ = \ EU \quad \text{and} \quad \mathbf{i}S\circ V \ = \ FV \tag{93}$$

for some antihermitian matrices E, F. Then

$$(\mathbf{i}R \circ U) \otimes (\mathbf{i}S \circ V) \;=\; -(R \otimes S) \circ (U \otimes V) \;=\; EU \otimes FV \;=\; (E \otimes F)(U \otimes V) \;, \tag{94}$$

from which we get

$$\mathbf{i}(R \otimes S) \circ (U \otimes V) \;=\; (-\mathbf{i}E \otimes F)(U \otimes V) \;, \tag{95}$$

where $(-\mathbf{i}E \otimes F)$ is antihermitian because $E \otimes F$ is hermitian. So $R \otimes S \in \mathbb{V}_{U \otimes V}$. ■

Therefore, if $\left(R_i^{(k)}\right)_{i=1..\mathbf{D}(U^{(k)})}$ are bases for $\mathbb{V}_{U^{(k)}}$, $k = 1..r$, then $R_{i_1}^{(1)} \otimes \ldots \otimes R_{i_r}^{(r)}$ form a set of $\mathbf{D}(U^{(1)}) \cdot \ldots \cdot \mathbf{D}(U^{(r)})$ independent vectors within $\mathbb{V}_{U^{(1)} \otimes \ldots \otimes U^{(r)}}$. Hence:

Corollary 3.6 *For a Kronecker product of unitaries (12) the generalized defect is supermultiplicative:*

$$\mathbf{D}\left(U^{(1)} \otimes \ldots \otimes U^{(r)}\right) \;\geq\; \mathbf{D}(U^{(1)}) \cdot \ldots \cdot \mathbf{D}(U^{(r)}) \tag{96}$$

The above mentioned set of $R_{i_1}^{(1)} \otimes \ldots \otimes R_{i_r}^{(r)}$ needs not to be a basis for $\mathbb{V}_{U^{(1)} \otimes \ldots \otimes U^{(r)}}$. For example, for the 2×2 unitary Fourier matrix:

$$F_2 \;=\; \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \tag{97}$$

we have that $\mathbf{D}(F_2 \otimes F_2) \;>\; \mathbf{D}(F_2) \cdot \mathbf{D}(F_2)$, as $\mathbf{D}(F_2 \otimes F_2) \;=\; 10$ and $\mathbf{D}(F_2) \;= 3$.

The space $\mathbb{V}_{U^{(k)}}$ constructed for a unitary $U^{(k)}$ of size $n_k \times n_k$ contains at least $2n_k - 1$ independent real matrices, denoted further by $R_i^{(k)}$, $i = 1..(2n_k - 1)$, which are all zero matrices except for the l-th row or m-th column filled all with ones, where $l = 1..n_k$ and $m = 2..n_k$. The corresponding directions $\mathbf{i}R_i^{(k)} \circ U^{(k)}$ were mentioned at (2) . Thus

$$\mathbf{D}\left(U^{(k)}\right) \;\geq\; 2n_k - 1 \;, \tag{98}$$

and consequently, by Corollary 3.6,

$$\mathbf{D}\left(U^{(1)} \otimes \ldots \otimes U^{(r)}\right) \;\geq\; (2n_1 - 1) \cdot \ldots \cdot (2n_r - 1) \;\;. \tag{99}$$

This is equal to (68), which is also valid if there is only one 2 in the sequence of sizes $(n_1, ..., n_r)$.

If there is more than one matrix of size 2×2 among $U^{(k)}$, in (99) we get a lower bound which is smaller than the lower bound (69). This is caused by the fact that, for x denoting the number of 2's in $(n_1, ..., n_r)$, there holds an equality for natural $x > 1$:

$$2^{x-1} \cdot (2^x + 1) \;>\; (2 \cdot 2 - 1)^x \;, \tag{100}$$

which is equivalent to

$$4^x - 3^x \;>\; 3^x - 2^x \;, \tag{101}$$

which in turn is true because, after dividing both sides by $(4-3) = (3-2) = 1$, on the left the summands are greater then on the right. So, in this situation, unsplitting the 2×2 matrices one by one from $U^{(1)}\otimes\ldots\otimes U^{(r)}$ is not a good strategy and it is better to write (by Corollary 3.6 and by (98)):

$$\mathbf{D}\left(U^{(1)}\otimes\ldots\otimes U^{(r)}\right) \;\geq\; \left(\prod_{n_k>2}\mathbf{D}\left(U^{(k)}\right)\right)\cdot\mathbf{D}\left(\bigotimes_{n_k=2}U^{(k)}\right) \;\geq\; \left(\prod_{n_k>2}(2n_k-1)\right)\cdot\mathbf{D}\left(\bigotimes_{n_k=2}U^{(k)}\right) \quad . \tag{102}$$

It would be interesting to conceive a set of $2^{x-1}(2^x+1)$ independent matrices of some elegant structure within $\mathbb{V}_{\bigotimes_{n_k=2}U^{(k)}}$, where x is the number of 2's in $(n_1,...,n_r)$, so that we could write (we can, but basing on Theorem 3.4):

$$\mathbf{D}\left(\bigotimes_{n_k=2}U^{(k)}\right) \;\geq\; 2^{x-1}\left(2^x+1\right) \quad . \tag{103}$$

(We mean here a guess similar to the above choice of $(2n_k-1)$ matrices $R_i^{(k)}$ in $\mathbb{V}_{U^{(k)}}$.) This, together with (102), would provide the bound (69) of Theorem 3.4, probably more directly than with the use of Theorems 3.2 and 2.6. Definitely, taking the 3^x matrices $\bigotimes_{n_k=2}R_{i_k}^{(k)}$, where factors come from the set

$$\left\{ \begin{bmatrix} 1 & 1\\ 0 & 0\end{bmatrix}, \begin{bmatrix} 0 & 0\\ 1 & 1\end{bmatrix}, \begin{bmatrix} 0 & 1\\ 0 & 1\end{bmatrix} \right\} \quad , \tag{104}$$

is, due to (100), not enough.

4 Conclusions

In this article we have achieved two things.

The first seems to be of great importance in numerical calculation of the defect (Definition 1.1) for large unitary $N\times N$ matrices U with a Kronecker product structure. This involves calculation of the dimension of a certain space $\mathbb{M}_U$ (defined in (9)), effectively in $\mathbb{R}^{N^2}$, spanned by the set $\mathcal{M}_U$ (defined in (10)), associated with U. It amounts to calculating the column rank of a certain matrix, call it $M(U)$, built on the entries of U, and can be performed for example by using rank/svd of MATLAB. When U has a Kronecker product structure, $\mathbb{M}_U$ can be split into a direct sum with a large number of components (see Theorem 2.6). So, instead of applying the procedure to $M(U)$ we can apply it to a number of its submatrices. This will make the whole calculation more reliable and may prevent divergence in svd used in calculation of the rank.

The second thing we have achieved in this work is the calculation, based on the above result, of the lower bound on the generalized defect $\mathbf{D}(U)$ (defined in (65), being the defect plus $2N-1$) when U is a Kronecker product. The generalized defect is supermultiplicative with respect to Kronecker subproducts of U (Corollary 3.6) and this allows us to trivially retrieve the lower bound of Theorem 3.4 when the number of 2×2 Kronecker factors does not exceed 1. In the other case Theorem 3.4 gives a better bound than that obtained using supermultiplicativity of $\mathbf{D}(U)$. We conjecture that, in either case, the lower bound is attained by most matrices with a fixed Kronecker product structure (fixed, up to an order, sequence of sizes of Kronecker factors).

All the formulas, the one expressing the direct sum forming $\mathbb{M}_U$ (see (52)), the resulting one expressing the dimension of $\mathbb{M}_U$ (see (57)), and the one expressing the lower bound (see (67), in a compact form (68) or (69)) are valid also when there are 1×1 Kronecker factors among those forming U, yielding the correct values we would get if the 1×1 factors were absorbed into larger factors. This property allows, in calculation of $\dim(\mathbb{M}_U)$ or its bound, the use of a procedure requiring a fixed number of factors, where the 1×1 [1]'s can be taken as potentially missing factors to extend a shorter Kronecker product.

The author believes that the first of the above mentioned achievements will open the way to easier calculation of the defect for large matrices U with a Kronecker product structure. Such calculations may be performed in order to asess whether a given U gives rise to a smooth family of inequivalent unitaries (i.e. not obtained one from another by multiplying rows and columns by unimodular numbers) with the moduli of entries fixed at the values sitting in $[|U_{i,j}|]_{i,j=1..N}$, and how large its dimension can be. This is a part of a question about unitary preimagies V to a doubly stochastic matrix $\left[|U_{i,j}|^2\right]_{i,j=1..N}$, that is about V such that $|V_{i,j}| = |U_{i,j}|$ for all i,j. This motivation is wider described in a prequel [1] to this paper. A special case, $\left[|U_{i,j}|^2\right]_{i,j=1..N} = [1/N]_{i,j=1..N}$, the search for complex Hadamard matrices, attracts even more interest, and it was dicussed in the Introduction.

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