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¹ The Group of Dyadic Unitary Matrices

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7 **Abstract.** We introduce the group DU(m) of $m \times m$ dyadic unitary matrices, i.e. unitary matrices with all entries having a real and an imaginary part that are both rational 8 numbers with denominator of the form 2^p (with p a non-negative integer). We investigate 9 in detail the finite groups DU(1) and DU(2) and the discrete, but infinite groups DU(3)10 and DU(4). We further introduce the subgroup XDU(m) of DU(m), consisting of those 11 members of DU(m) that have constant line sum 1. The study of XDU(2) and XDU(4)12 leads to conclusions concerning the synthesis of quantum computers acting on one and two 13 qubits, respectively. 14

1. Introduction

- ¹⁶ Basically, there exist three kinds of groups:
- finite groups, i.e. groups with a finite order,
- infinite but nevertheless discrete groups, i.e. groups with a countably
 infinite order, and
- Lie groups, i.e. groups with an uncountably infinite order.

Whereas the size of a finite group is quantified by its order, the size of a Lie 21 group is quantified by its dimensionality. Quantifying sizes of infinite discrete 22 groups is a more difficult task. It necessitates a detailed study of the group. 23 The most basic example of a countably infinite nonabelian group is the 24 discrete group $SL_2(\mathbb{Z})$, i.e. the special linear group of 2×2 matrices with in-25 teger entries. Conrad [1] demonstrates that the group can be generated with 26 merely two generators and shows how to decompose an arbitrary group mem-27 ber into a finite product of factors, each equal to one of these two building 28 blocks. In the present paper, we follow a basically similar approach for de-29 scribing the group of rational unitary matrices where all matrix elements have 30 a denominator of the form 2^p . The motivation to study this group is inspired 31 32 by its importance in computer theory. Whereas classical reversible computation is described by finite groups and quantum computation is represented by 33

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Lie groups, computing with the so-called square-root-of-NOT logic gate leads to infinite discrete groups [2] of such rational matrices. Whereas classical reversible circuits are generated by controlled NOT gates (a.k.a. Toffoli gates), below we will investigate all circuits generated by controlled square roots of NOT. They constitute a generalization of the classical reversible circuits, but only a small fraction of the set of all quantum circuits.

2. The Group DU(m)

First, we consider all unitary $m \times m$ matrices. It is well known that they form an infinite group, i.e. the unitary group U(m), an m^2 -dimensional Lie group.

Next, we consider, within the group U(m), the matrices which have exclusively Gaussian entries. This means that the matrix entries are Gaussian rationals

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$$\frac{a}{A} + i \frac{b}{B}, \quad \frac{c}{C} + i \frac{d}{D}, \quad \dots$$

where a, A, b, B, \ldots are integers. These matrices form a group. Indeed, being unitary, such matrix has an inverse. The entries of the inverse automatically are also Gaussian rationals. And the product of two such matrices automatically is also such a matrix. We call this group the Gaussian unitary group GU(m). The group is discrete, as the matrix contains only a finite number (i.e. $2m^2$) of rational numbers $\frac{a}{A}, \frac{b}{B}, \ldots$ and there exist only a countably infinite number of rationals.

Finally, within the group GU(m), we consider the subset of matrices where all denominators A, B, \ldots are a power of 2. Thus all entries may be written

58
$$\frac{a}{2^p} + i \frac{b}{2^p}$$

where the non-negative integer p is chosen such that at least one entry is not reducible, i.e. such that at least one of the $2m^2$ numerators a, b, \ldots is odd. As the real part and the imaginary part of each matrix entry is a dyadic rational, we call such a matrix a dyadic matrix. Whereas m is called the dimension (or degree) of the matrix, the number 2^p is called the level [3] of the matrix. As illustrated by the example

$$\begin{pmatrix} \frac{5}{2} & 1\\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}^{-1} = \begin{pmatrix} \frac{2}{3} & -\frac{4}{3}\\ -\frac{2}{3} & \frac{10}{3} \end{pmatrix},$$

the inverse of a dyadic matrix is not necessarily a dyadic matrix. The inverse of dyadic unitary matrix, however, is a dyadic unitary matrix (with the same level), for the simple reason that the inverse of a unitary matrix is its Hermitian transpose. The product of a dyadic matrix with level equal to 2^{p_1} and a ⁷⁰ dyadic matrix with level equal to 2^{p_2} is a dyadic matrix with level lower than ⁷¹ or equal to $2^{p_1+p_2}$. We thus may conclude that the dyadic unitary matrices ⁷² form a group. We call this group the dyadic unitary group DU(m).

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3. Two Subgroups of DU(m)

In the present section, we discuss two (out of the many) subgroups of DU(m). 74 An $m \times m$ matrix has 2m lines, i.e. m rows and m columns. We consider 75 the matrices whose line sums are all equal. If the matrix is unitary, then 76 the constant line sum is on the unit circle (See Appendix A). If the matrix is 77 dyadic, then the constant line sum is a dyadic rational. Now, on the unit circle 78 there exist only four such Gaussian rationals $\frac{x}{2^p} + i \frac{y}{2^p}$. Indeed, the condition $(\frac{x}{2^p})^2 + (\frac{y}{2^p})^2 = 1$ leads to $x^2 + y^2 = (2^p)^2$, which implies that $\{x, y, 2^p\}$ forms 79 80 a Pythagorean triple. However, there exist no primitive Pythagorean triples 81 where the greatest number is even. We conclude that either x or y has to 82 be zero. Therefore, if the matrix is both unitary and dyadic, the constant 83 line sum equals one of the four complex numbers 1, i, -1, and -i, known 84 as the four Gaussian units. The product of a matrix with constant line sum 85 equal to s and a matrix with constant line sum equal to t is a matrix with 86 constant line sum st. Proof is provided in [4, p. 239]. Therefore, matrices 87 with constant line sum equal to 1 form a group. The members of DU(m) that 88 have constant line sum equal to 1, thus form a subgroup of DU(m); we will 89 call this subgroup XDU(m). Their study is interesting in the framework of 90 quantum computing. The groups $XDU(2^w)$ naturally appear when studying 91 quantum circuits built with the gate called 'the square root of NOT', see below 92 in Sections 8 to 11. Matrices belonging to XDU(m) may be considered as 93 a 'complex generalization' of doubly stochastic (or bistochastic) matrices, 94 where equally well all line sums equal 1, but where all entries are restricted 95 to real non-negative numbers. 96

The matrices of DU(m) with p = 0, i.e. the DU(m) matrices of level 1, form a finite subgroup, isomorphic to the semi-direct product $(DU(1) \times$ $DU(1) \times \ldots \times DU(1)$): $S_m = DU(1)^m : S_m$, where S_m denotes the symmetric group of degree m (and thus order m!). We will call the subgroup the monomial dyadic unitary group MDU(m), as all its members are matrices with exactly one non-zero entry in each row and each column. The group P(m) of all $m \times m$ permutation matrices, in turn, is a subgroup of MDU(m):

104
$$P(m) \subset MDU(m) \subset DU(m) \subset U(m).$$

The subgroup MDU(m) partitions the supergroup DU(m) into double cosets, each containing matrices of a same level 2^p . These double cosets can be regarded as equivalence classes. Any element of a double coset can act as its representative. Here, two matrices are considered equivalent iff they can

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¹⁰⁹ be converted into one another by applying a combination of the following¹¹⁰ operations:

- permutation of two rows or two columns and
- multiplication of a row or a column by *i*.

This equivalence is analogous to the one used in investigating real and complex Hadamard matrices. See e.g. the equivalence relation \approx by Haagerup [5].

4. The Group DU(1) and its subgroup XDU(1)

The group DU(1) is the group of Gaussian numbers $\frac{a}{2^p} + i\frac{b}{2^p}$, such that $(\frac{a}{2^p})^2 + (\frac{b}{2^p})^2 = 1$. As demonstrated in the previous section, only the numbers ± 1 and $\pm i$ satisfy this condition. Thus DU(1) is isomorphic to the finite group of the four complex numbers 1, i, -1, and -i. This group has order 4 and is isomorphic to the cyclic group \mathbb{Z}_4 .

The subgroup MDU(1) is identical to DU(1). The subgroup XDU(1) has order 1 and is isomorphic to Z_1 .

5. The Group DU(2) and its Subgroup XDU(2)

¹²⁴ We consider the unitary matrices of the form

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$$\begin{pmatrix} \frac{a}{2^p} + i \frac{b}{2^p} & \frac{c}{2^p} + i \frac{d}{2^p} \\ \frac{e}{2^p} + i \frac{f}{2^p} & \frac{g}{2^p} + i \frac{h}{2^p} \end{pmatrix},$$

where at least one of the eight integers a, b, c, \ldots, h is odd. For the sake of convenience, we assume that $\{a, b, c, d\}$ contains an odd number. We have

$$a^2 + b^2 + c^2 + d^2 = 4^p.$$
(1)

According to Lagrange's theorem each natural number can be written as the sum of four squares. So can 4^p .

If p = 0, then only one partition into four squares exists:

132
$$1 = 1^2 + 0^2 + 0^2 + 0^2$$
. (2)

If p > 0, then (1) implies that $a^2 + b^2 + c^2 + d^2$ has to be a multiple of 4. Therefore, either all four numbers a, b, c, and d are even or all are odd. If p = 1, then both kinds of partition exist:

136
$$4 = 1^{2} + 1^{2} + 1^{2} + 1^{2}$$
(3)
137
$$= 2^{2} + 0^{2} + 0^{2} + 0^{2}.$$

4

138 If p > 1, then the four numbers are necessarily even:

139
$$4^{p} = (2^{p-1})^{2} + (2^{p-1})^{2} + (2^{p-1})^{2} + (2^{p-1})^{2}$$

140 =
$$(2^p)^2 + 0^2 + 0^2 + 0^2$$

We denote by $p_s(n)$ the number of partitions of a number n into s squares. 141 In contrast to this number of partitions, the total number of representations 142 of the number n as a sum of s squares takes into account order and sign of 143 the parts, thus e.g. considering $4 = 2^2 + 0^2 + 0^2 + 0^2$, $4 = 0^2 + 2^2 + 0^2 + 0^2$, and 144 $4 = (-2)^2 + 0^2 + 0^2 + 0^2$ as three different solutions of $a^2 + b^2 + c^2 + d^2 = 4$. 145 This number of 'lattice on the hypersphere with radius \sqrt{n} ' traditionally is 146 denoted $r_s(n)$. We have (for n > 0 and s > 3) that $r_s(n) \gg p_s(n)$. Thanks 147 to Jacobi [6], explicit expressions [7, 8, 9] exist for $r_2(n)$, $r_4(n)$, $r_6(n)$, $r_8(n)$, 148 and $r_{12}(2n)$. In particular, we have 149

150
$$r_4(n) = 8 \sum_{4 \not\mid d \mid n} d,$$

151 yielding

152

154

165

$$r_4(4^p) = \begin{cases} 8 & \text{if } p = 0\\ 24 & \text{if } p > 0. \end{cases}$$
(4)

153 As a result, we have

$$p_4(4^p) = \begin{cases} 1 & \text{if } p = 0\\ 2 & \text{if } p > 0 \end{cases}$$

Thus there exist no other partitions of 4^p than those mentioned above. As a result, there exists no partition $a^2 + b^2 + c^2 + d^2$ of 4^p (with p > 1) with at least one odd number a, b, c, or d. That is the reason why there do not exist any dyadic unitary 2×2 matrices with $p \ge 2$. The fact that neither $p_4(4^p)$ nor $r_4(4^p)$ increase for increasing p, once $p \ge 1$, explains why no dyadic unitary 2×2 matrices with p > 1 exist.

We conclude that the group DU(2) consists of matrices with level equal to either 1 or 2. As a consequence, the group is finite. It consists of the Gaussian unitary matrices where either all denominators are 1 (and numerators are based on (2)) or all denominators are 2 (and numerators are based on (3)):

$$\left(\begin{array}{cc} \alpha & 0 \\ 0 & \beta \end{array}\right) \text{ or } \left(\begin{array}{cc} 0 & \alpha \\ \beta & 0 \end{array}\right) \text{ or } \frac{1}{2} \left(\begin{array}{cc} a+ib & c+id \\ e+if & g+ih \end{array}\right),$$

where α and β are 1, i, -1, or -i and a, b, \ldots , and h are 1 or -1. This yields a group of order 96. Its most notorious members are

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$
, $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and $\frac{1}{2} \begin{pmatrix} 1+i & 1-i \\ 1-i & 1+i \end{pmatrix}$

representing, in quantum computation, the dummy gate, the NOT gate [10, 4], 166 and the square root of NOT gate [2, 10, 4, 11, 12, 13], respectively. The group 167 is isomorphic to the group [96, 67] of the GAP library. It consists of 32 168 matrices with p = 0 and 64 matrices with p = 1. The former constitute 169 the subgroup MDU(2), isomorphic to $(DU(1) \times DU(1))$: S_2 and thus to 170 \mathbf{Z}_4^2 : \mathbf{Z}_2 . The subgroup MDU(2) partitions the supergroup DU(2) into two 171 double cosets, one containing all the matrices with p = 0, the other all the 172 matrices with p = 1. 173

Besides the permutation group P(2), also the Pauli group [14, 15] P is a subgroup of MDU(2):

176
$$P(2) \subset \boldsymbol{P} \subset MDU(2) \subset DU(2) \subset U(2),$$

177 with successive orders

$$4 < 16 < 32 < 96 < \infty^4.$$

According to the definition in Sect. 3, the members of DU(2) with all four line sums equal to 1, form the subgroup XDU(2) of DU(2). The subgroup has order 4. Only two of the four matrices of XDU(2) belong to MDU(2). The subgroup XDU(2) partitions its supergroup DU(2) into nine double cosets, five of size 16 and four of size 4.

For the case m = 3, we have to investigate a partition into six squares:

186
$$a^2 + b^2 + c^2 + d^2 + e^2 + f^2 = 4^p$$

with at least one of the integers $\{a, b, c, d, e, f\}$ odd. Whatever the value of p, such partition is possible. Suffice it to successively

• choose an arbitrary odd number a such that $a^2 \leq 4^p$,

• choose an arbitrary number b such that $b^2 \leq 4^p - a^2$, and

• apply Lagrange's four-square theorem to the number $4^p - a^2 - b^2$.

¹⁹² There always exists at least one partition of the form

193
$$4^p = 1^2 + 0^2 + c^2 + d^2 + e^2 + f^2.$$

As p can have any value from $\{0, 1, 2, ...\}$, this yields a (countably) infinite number of possibilities. This fact constitutes the underlying reason why DU(3) (in contrast to DU(2)) is a (countably) infinite group. An actual proof of the infinitude of DU(3) is given in Appendix B. The numbers $p_6(4^p)$ and $r_6(4^p)$ grow fast with increasing p. Indeed, according to Jacobi, we have

200
$$r_6(n) = 4 \sum_{2 \not\mid d \mid n} (-1)^{(d-1)/2} \left(\frac{4n^2}{d^2} - d^2 \right).$$

201 For $n = 4^p$ this yields

202
$$r_6(4^p) = 4(4 \times 16^p - 1),$$

i.e. an exponentially increasing function of p, in strong contrast to (4).

Within the infinite group DU(3), the matrices with p = 0 form the finite subgroup MDU(3), isomorphic to $(DU(1) \times DU(1) \times DU(1)) : S_3$, of order $4^3 \times 3! = 384$. It partitions the whole group into an infinite number of double cosets. All elements of such a double coset have a same value of p. However, two matrices with a same p may be member of two different double cosets. E.g. the two matrices

$${}_{210} \qquad \frac{1}{2^2} \left(\begin{array}{cccc} 1 & 1+2i & 3-i \\ -3-2i & 1 & 1+i \\ 1-i & -1-3i & 2 \end{array} \right) \text{ and } \frac{1}{2^2} \left(\begin{array}{cccc} -3+i & 1+i & 2 \\ 1+i & -3+i & 2 \\ 2 & 2 & 2+2i \end{array} \right)$$

sit in two different double cosets, both with p = 2. The former double coset contains matrices, where all lines (i.e. rows and columns) are based on the partition $16 = 3^2 + 2^2 + 1^2 + 1^2 + 1^2 + 0^2$. The latter double coset contains matrices where four lines are based on this partition, but two other lines are based on $16 = 2^2 + 2^2 + 2^2 + 2^2 + 0^2 + 0^2$. The two double cosets have different size: the former contains $36,864 = 96 \times 384$ elements, whereas the latter contains only $18,432 = 48 \times 384$ elements.

For large values of n, we have

219
$$p_s(n) \, pprox \, rac{r_s(n)}{s! \, 2^s} \, ,$$

such that, for sufficiently large p, we have

221
$$p_6(4^p) \approx \frac{1}{2880} 16^p$$

The fact that $p_6(4^p)$ grows so rapidly with increasing p leads to a fast growing number of double cosets as a function of the level 2^p . For p = 1, we have two double cosets; for p = 2, we have six double cosets; and for p = 3, we have at least seven double cosets. The two double cosets with p = 1 have e.g. the following representatives:

$$r_{1} = \frac{1}{2} \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1+i & 1-i \\ 0 & 1-i & 1+i \end{pmatrix} \text{ and } r_{2} = \frac{1}{2} \begin{pmatrix} 0 & 1-i & 1+i \\ 1+i & 1 & -i \\ 1-i & i & 1 \end{pmatrix},$$

| | m = 1 | m = 2 | m = 3 | m = 4 | |
|---------------|-------|-------|-----------------|-------------|--|
| p = 0 $q = 0$ | 4 | 32 | 384 | 6,144 | |
| p=1 $q=1$ | 0 | 64 | $2,\!304$ | $147,\!456$ | |
| p=1 $q=2$ | 0 | 0 | 9,216 | 5,701,632 | |
| p = 2 $q = 3$ | 0 | 0 | $36,\!864$ | | |
| p = 2 $q = 4$ | 0 | 0 | $147,\!456$ | | |
| p=3 $q=5$ | 0 | 0 | 589,824 | | |
| p = 3 $q = 6$ | 0 | 0 | $2,\!359,\!296$ | | |
| | | | | | |
| total | 4 | 96 | \aleph_0 | $leph_0$ | |

Table 1: Number of DU(m) matrices.

²²⁸ respectively.

It turns out to be advantageous to decompose the number 2 into the irreducible elements of the Gaussian integers,

231 $2 = -i(1+i)^2$,

where -i is one of the four Gaussian units (i.e. 1, i, -1, and -i) and 1+i is a Gaussian prime. We thus obtain

$$r_{1} = \frac{1}{1+i} \begin{pmatrix} 1+i & 0 & 0\\ 0 & i & 1\\ 0 & 1 & i \end{pmatrix}, \quad r_{2} = \frac{1}{(1+i)^{2}} \begin{pmatrix} 0 & 1+i & i(1+i)\\ i(1+i) & i & 1\\ 1+i & -1 & i \end{pmatrix}.$$

We may say that r_1 is of level 1+i, whereas r_2 is of level $(1+i)^2$. In this sense, 235 the matrices of level 2^p consist of the union of the matrices of level $(1+i)^{2p-1}$ 236 and the matrices of level $(1+i)^{2p}$. We may say that the Gaussian prime 1+i237 plays a role like 'some kind of rational square root of 2', thus allowing levels 238 resembling a 'halfinteger power of 2'. We will use χ as a short-hand notation 239 for 1 + i. We will make use of the following property of the number χ : any 240 Gaussian integer is either $0 \mod \chi$ or $1 \mod \chi$. A Gaussian number a + ib is 241 $0 \mod \chi$ iff either both a and b are even or both a and b are odd. 242

The number of DU(3) matrices of different levels χ^q are given in Table 1. All matrices of level χ^0 are members of MDU(3), a group isomorphic to DU(1)³: **S**₃ of order 4³×3! = 384. All 3×3 matrices of level χ^1 consist of a 1× 1 DU(1) block (4 possible contents) and a 2×2 DU(2) block (64 possibilities), with 9 possible block placings: indeed we have $9 \times (4 \times 64) = 2,304$. All matrices of level χ^2 or higher do not fall apart into blocks. Table 1 reveals that, for q > 0, the number of DU(3) matrices with level χ^q equals 576 × 4^q. Appendix C explains why. For p > 0, the DU(3) matrices of level 2^p consist of the matrices of levels χ^{2p-1} and χ^{2p} . Thus (for p > 0) there are 720 × 16^p such matrices.

An arbitrary matrix A of DU(3) of level χ^q looks like

$$A = \frac{1}{\chi^q} \begin{pmatrix} a+ib & c+id & e+if \\ g+ih & j+ik & l+im \\ n+io & p+iq & r+is \end{pmatrix}$$
(5)

with at least one of the nine entries a + ib, c + id, ..., or r + is not divisible by χ . We now introduce the matrix $R_n(A)$, where n is a Gaussian integer. It is obtained by multiplying A by its level χ^q and subsequently computing the remainder when dividing each matrix entry by n:

$$R_n(A) = (\chi^q A) \mod n.$$

260 E.g.

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254

$$R_{\chi} \left[\frac{1}{(1+i)^5} \begin{pmatrix} 4+2i & 1-3i & -1-i \\ -1+3i & -3 & -3+2i \\ 1-i & 2+3i & -4-i \end{pmatrix} \right] = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix}$$

$$R_{2} \left[\frac{1}{(1+i)^5} \begin{pmatrix} 4+2i & 1-3i & -1-i \\ -1+3i & -3 & -3+2i \\ 1-i & 2+3i & -4-i \end{pmatrix} \right] = \begin{pmatrix} 0 & 1+i & 1+i \\ 1+i & 1 & 1 \\ 1+i & i & i \end{pmatrix}$$

Note that all entries of an R_{χ} matrix are either 0 or 1 and all entries of an R_2 matrix are 0, 1, *i*, or 1 + i.

For any Gaussian integer n, we have $n\overline{n} \mod \chi = n \mod \chi$. Therefore, the unitarity condition

$$a^2 + b^2 + c^2 + d^2 + e^2 + f^2 = 2^q$$
,

in case q > 0, leads to

$$(a+ib) \mod \chi + (c+id) \mod \chi + (e+if) \mod \chi = 0$$

and similar for the remaining two rows, as well as for the three columns. Taking also orthogonalities into account, we can conclude that the R_{χ} matrix of a DU(3) matrix (of level higher than 1) always is of the type

273
$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix}$$
(6)

or equivalent, i.e. of this type after permutation of rows or permutation of columns. One can similarly demonstrate that the R_2 matrix of a DU(3) matrix (of level higher than χ^1) always is of the following type or equivalent:

$$\begin{pmatrix} 0 & 1+i & 1+i \\ 1+i & M \\ 1+i & M \end{pmatrix},$$
(7)

where the lower-right submatrix M exists in five flavours:

279
$$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 1 \\ i & i \end{pmatrix}, \begin{pmatrix} 1 & i \\ 1 & i \end{pmatrix}, \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}$$
 and $\begin{pmatrix} i & i \\ i & i \end{pmatrix}$.

They correspond to the five 2×2 matrices G_1, G_2, \ldots , and G_5 discussed in Appendix D.

By multiplying the DU(3) matrix of level χ^q by an appropriate DU(3) matrix of level χ , it always is possible to obtain a matrix of level χ^{q-1} (instead of level χ^{q+1} , as one would expect normally). By performing such a multiplication again and again, we can thus lower the level of the matrix from χ^q to χ^{q-1} , to χ^{q-2} , ..., to χ^0 . It suffices to proceed, at each of the q stages, in three steps:

• First, one multiplies by an appropriate permutation matrix (automatically of level 1), such that the original R_{χ} matrix is converted into the standard form (6).

$$b = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -i & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Detailed study [16] demonstrates that the b matrix has to be applied if the R_2 matrix (7) contains the submatrix

295
$$\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 1 \\ i & i \end{pmatrix}$$
 or $\begin{pmatrix} i & i \\ i & i \end{pmatrix}$

and the b matrix should not be applied if the submatrix is

296

297

either
$$\begin{pmatrix} 1 & i \\ 1 & i \end{pmatrix}$$
 or $\begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}$.

• Finally, one right-multiplies by the matrix (of level χ)

$$a = \frac{1}{2} \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1-i & 1+i \\ 0 & 1+i & 1-i \end{pmatrix} = \frac{1}{1+i} \begin{pmatrix} 1+i & 0 & 0 \\ 0 & -i & 1 \\ 0 & 1 & -i \end{pmatrix}.$$

The second and the third step of the procedure are illustrated by an example where we lower the level of a given matrix from χ^5 to χ^4 :

$$302 \qquad \frac{1}{(1+i)^5} \begin{pmatrix} 4+2i & 1-3i & -1-i \\ -1+3i & -3 & -3+2i \\ 1-i & 2+3i & -4-i \end{pmatrix} b a = \frac{1}{(1+i)^4} \begin{pmatrix} 3-i & -1+i & -2 \\ 1+2i & i & 1+3i \\ -i & -3-2i & 1+i \end{pmatrix},$$

³⁰³ what, expressed in dyadic form, looks like

$${}_{304} \quad \frac{1}{8} \left(\begin{array}{cccc} -6+2i & 2+4i & 2\\ -2-4i & 3-3i & 1-5i\\ 2i & -5-i & 5-3i \end{array} \right) b \, a \ = \ \frac{1}{4} \left(\begin{array}{cccc} -3+i & 1-i & 2\\ -1-2i & -i & -1-3i\\ i & 3+2i & -1-i \end{array} \right).$$

The underlying reason why the 3-step procedure always works, is explained in Appendix D: it suffices to choose the appropriate matrix

$$c = \left(\begin{array}{cc} c_{11} & c_{12} \\ c_{21} & c_{22} \end{array}\right),$$

equal either to

$$\frac{1}{2} \begin{pmatrix} 1-i & 1+i \\ 1+i & 1-i \end{pmatrix} \quad \text{or to} \quad \begin{pmatrix} -i & 0 \\ 0 & 1 \end{pmatrix} \frac{1}{2} \begin{pmatrix} 1-i & 1+i \\ 1+i & 1-i \end{pmatrix},$$

 $_{305}$ in order to guarantee that the product of two R_2 matrices

$$\begin{pmatrix} 0 & 1+i & 1+i \\ 1+i & g_{11} & g_{12} \\ 1+i & g_{21} & g_{22} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_{11} & c_{12} \\ 0 & c_{21} & c_{22} \end{pmatrix}$$

is the 3×3 zero matrix (modulo 2). Now, if an $R_2(A)$ matrix is the zero matrix, then all entries of matrix A are divisible by 2 (and therefore by χ^2). By applying the procedure again and again, we eventually obtain a decomposition of an arbitrary matrix into

•
$$q$$
 matrices $a^{-1} = \frac{1}{2} \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1+i & 1-i \\ 0 & 1-i & 1+i \end{pmatrix}$,
112 • q or less matrices $b^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & i & 0 \\ 0 & 0 & 1 \end{pmatrix}$,

• q + 1 permutation matrices, and

• one diagonal matrix,

315 e.g.

$$\frac{1}{8} \begin{pmatrix} -6+2i & 2+4i & 2\\ -2-4i & 3-3i & 1-5i\\ 2i & -5-i & 5-3i \end{pmatrix}$$

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322

$$= \begin{pmatrix} -i & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} a^{-1} b^{-1} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} a^{-1} b^{-1} \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} a^{-1} \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} a^{-1} \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} a^{-1} b^{-1}.$$

No procedure for shorter decomposition into matrices of levels 1 and χ is pos-319 sible. Multiplication by a level- χ matrix indeed cannot convert an arbitrary 320 matrix of level χ^q into a matrix of level χ^{q-2} . 321

The Subgroup XDU(3) 7.

The members of DU(3) with all six line sums equal to 1 form the infinite 323 subgroup XDU(3) of DU(3). Any line of an XDU(3) matrix is, just like any 324 line of a DU(3) matrix, based on a partition into six squares: 325

326
$$a^2 + b^2 + c^2 + d^2 + e^2 + f^2 = 4^p$$

however with the two additional restrictions: 327

328
$$a + c + e = 2^p$$

329 $b + d + f = 0$.

The number of integer solutions therefore is much smaller than $r_6(4^p)$. Find-330 ing the exact number of solutions is no easy problem. It turns out to be equal 331 to $3(2 \times 4^p - 1)$, according to [17]. 332

Just like DU(3), we subdivide XDU(3) either into classes of different 333 level 2^p or into classes of different level $(1+i)^q$. The matrices of level 1 334 form a subgroup: the 3! permutation matrices. This subgroup P(3) divides 335 the supergroup XDU(3) into double cosets. There exist two double cosets of 336 level 2, with representatives r_1 and 337

$$\frac{1}{2} \begin{pmatrix} 1 & i & 1-i \\ -i & 1 & 1+i \\ 1+i & 1-i & 0 \end{pmatrix}$$

and with sizes 18 and 36, respectively. The former is of level $(1 + i)^1$, the 339 latter of level $(1+i)^2$. See Table 2. We note that, for q > 1, the number of 340 double cosets equals 2^{q-2} , each set being of size 36, such that the number of 341 matrices equals 9×2^{q} . This is demonstrated in Appendix C.1. The XDU(3) 342 matrices of level 2^p consist of the matrices of levels $(1+i)^{2p-1}$ and $(1+i)^{2p}$. 343 Therefore, there are $\frac{27}{2} 4^p$ such matrices. 344

While applying the 3-step DU(3) matrix decomposition method to an 345 XDU(3) matrix, one automatically obtains a product without any diagonal 346

12

(-i)

| | m = 1 | m = 2 | m = 3 | m = 4 | |
|--|--|----------|---|--------------------|--|
| p = 0 q = 0 |) 1 | 2 | 6 | 24 | |
| $\begin{vmatrix} p = 1 & q = 1 \\ p = 1 & q = 2 \end{vmatrix}$ | $ \begin{array}{c ccccccccccccccccccccccccccccccccccc$ | $2 \\ 0$ | $\frac{18}{36}$ | $216 \\ 2,256$ | |
| $\begin{vmatrix} p=2 & q=2\\ p=2 & q=2 \end{vmatrix}$ | $\begin{array}{c c}3 & 0\\4 & 0\end{array}$ | 0 0 | $\begin{array}{c} 72\\144\end{array}$ | $16,320 \\ 57,600$ | |
| $\begin{vmatrix} p = 3 & q = 0 \\ p = 3 & q = 0 \end{vmatrix}$ | 5 0 5 0 | 0 0 | $\begin{array}{c} 288 \\ 576 \end{array}$ | 230,400 921,600 | |
| $\begin{vmatrix} p = 4 & q = 0 \\ p = 4 & q = 0 \end{vmatrix}$ | 7 0 8 0 | 0 0 | $1,152 \\ 2,304$ | | |
| total | 1 | 4 | \aleph_0 | $leph_0$ | |

Table 2: Number of XDU(m) matrices.

matrices: the second step of the 3-step procedure thus is absent, such that
all factors of the decomposition belong to XDU(3). The underlying reason is
given at the end of Appendix D. As an example, we have

$$\frac{1}{8} \begin{pmatrix} 1-3i & 1+4i & 6-i \\ 6+4i & 1-i & 1-3i \\ 1-i & 6-3i & 1+4i \end{pmatrix} = p_1 a^{-1} p_2 a^{-1} p_3 a^{-1} p_$$

where the 3×3 matrices a and a^{-1} are defined in Sect. 6 and where

$$p_1 = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad p_2 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad p_3 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}.$$

Because the group P(3) of permutations can be generated by two generators, e.g.

$$\begin{array}{ccc} 355 \\ \end{array} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \\ \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \\ \end{pmatrix},$$

 $_{\rm 356}$ $\,$ and because

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} = (a^{-1})^2,$$

10

0.

1

we may conclude that the group XDU(3) can be generated by two generators, e.g.

$$g_1 = \frac{1}{2} \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1+i & 1-i \\ 0 & 1-i & 1+i \end{pmatrix} \quad \text{and} \quad g_2 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}.$$

0

³⁶¹ Finally, because

10

0

$$g_{2} = \frac{1}{2} \begin{pmatrix} 1+i & 0 & 1-i \\ 0 & 2 & 0 \\ 1-i & 0 & 1+i \end{pmatrix} \frac{1}{2} \begin{pmatrix} 1+i & 0 & 1-i \\ 0 & 2 & 0 \\ 1-i & 0 & 1+i \end{pmatrix} \times \frac{1}{2} \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1+i & 1-i \\ 0 & 1-i & 1+i \end{pmatrix} \frac{1}{2} \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1+i & 1-i \\ 0 & 1-i & 1+i \end{pmatrix},$$

364 XDU(3) can also be generated by the following two generators:

$$\frac{1}{2} \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1+i & 1-i \\ 0 & 1-i & 1+i \end{pmatrix} \quad \text{and} \quad \frac{1}{2} \begin{pmatrix} 1+i & 0 & 1-i \\ 0 & 2 & 0 \\ 1-i & 0 & 1+i \end{pmatrix}.$$

Thus any member of XDU(3) can be written as a product of square roots of 3×3 permutation matrices.

8. The Group
$$DU(4)$$

369 Jacobi's formula

$$r_8(n) = 16 (-1)^n \sum_{d \mid n} (-1)^d d^3$$

371 yields

368

370

$$r_8(4^p) = \begin{cases} 16 & \text{if } p = 0\\ \frac{16}{7} (8 \times 64^p - 15) & \text{if } p > 0, \end{cases}$$

 $_{373}$ such that it is no surprise DU(4) is infinite.

We consider within the infinite group DU(4), the subgroup MDU(4) of 374 monomial matrices. It is isomorphic to $DU(1)^4$: S_4 , of order $4^4 \times 4! = 6, 144$. 375 Twenty-four of its members are permutation matrices and thus represent 376 the 24 classical reversible logic circuits acting on two bits. The monomial 377 subgroup partitions the total group into an infinite number of double cosets. 378 All matrices of m = 4 and p = 1 have at least one line based on the 379 partition $4 = 1^2 + 1^2 + 1^2 + 1^2 + 0^2 + 0^2 + 0^2 + 0^2$, the remaining lines being based on $4 = 2^2 + 0^2 + 0^2 + 0^2 + 0^2 + 0^2 + 0^2 + 0^2 + 0^2$. One of the double cosets 380 381 contains the two square roots of NOT, such as 382

$${}^{_{383}} \qquad \qquad \frac{1}{2} \left(\begin{array}{cccc} 1+i & 1-i & 0 & 0\\ 1-i & 1+i & 0 & 0\\ 0 & 0 & 1+i & 1-i\\ 0 & 0 & 1-i & 1+i \end{array} \right)$$



Fig. 1: From left to right: two square roots of NOT, four controlled square roots of NOT, and the twin square roots of NOT.

Its size is 73,728. Another double coset (equally of size 73,728) contains the four controlled square roots of NOT, such as^a

$$\frac{1}{2} \left(\begin{array}{rrrr} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1+i & 1-i \\ 0 & 0 & 1-i & 1+i \end{array} \right)$$

386

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See Fig. 1. All six circuits belong to XDU(4). Both double cosets have level 1+i.

There exist 393,216 unitary matrices where all entries are from the set of the 4 numbers $\frac{1}{2}$ {1, *i*, -1, -*i*}. These matrices are of the form $\frac{1}{2}$ *H*(4, 4), where *H*(4, 4) denotes the 4×4 complex (or: generalized) Hadamard matrices [18]. They fall apart into two equivalence classes: 294,912 are represented by the dephased matrix

$${}^{394} \qquad \qquad \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{pmatrix}, \tag{8}$$

i.e. 1/2 times the 4-point Fourier transform F_4 ; the 98,304 remaining matrices being represented by the dephased matrix

i.e. the tensor product of two 2-point Fourier transforms F_2 :

$$\frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

400 To the latter double coset belongs the matrix representing the twin square

^aA 'controlled square root of NOT' may also be called a 'square root of controlled NOT', as well as a 'square root of Feynman gate'.

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401 roots of NOT:

$${}^{402} \qquad \frac{1}{2} \left(\begin{array}{ccc} 1+i & 1-i \\ 1-i & 1+i \end{array} \right) \otimes \frac{1}{2} \left(\begin{array}{ccc} 1+i & 1-i \\ 1-i & 1+i \end{array} \right) = \frac{1}{2} \left(\begin{array}{ccc} i & 1 & 1 & -i \\ 1 & i & -i & 1 \\ 1 & -i & i & 1 \\ -i & 1 & 1 & i \end{array} \right).$$

All matrices of the form $\frac{1}{2} H(4,4)$ are of level $(1+i)^2$.

The above-mentioned four double cosets (containing a total of 540,672 matrices) do not exhaust all unitary dyadic matrices with p = 1, as is illustrated by the existence of e.g.

407
$$\frac{1}{2} \begin{pmatrix} 1+i & 1 & 1 & 0\\ 1+i & -1 & -1 & 0\\ 0 & 1 & -1 & 1+i\\ 0 & -1 & 1 & 1+i \end{pmatrix}.$$

⁴⁰⁸ There are in fact nine classes [16] with level 2^1 .

All matrices of level $(1+i)^0$ fall apart in four 1×1 blocks and are member 409 of the MDU(4) subgroup of DU(4): we have $24 \times 4^4 = 6,144$ such matrices. 410 All matrices of level $(1 + i)^1$ either consist of two DU(1) blocks and one 411 DU(2) block or consist of two DU(2) blocks. We have $72 \times (4^2 \times 64) + 18 \times 64^2 =$ 412 147,456 such matrices. Among the 5,701,632 matrices of level $(1+i)^2$, there 413 are $16 \times (4 \times 9, 216) = 589,824$ ones, which consist of one DU(1) block and 414 one DU(3) block. All the matrices of level $(1 + i)^3$ or higher do not have 415 a block structure. Finally, Table 1 gives the number of DU(4) matrices for 416 some levels. 417

Whereas m = 3 leads to only one matrix type modulo χ , i.e. the matrix type (6), the case m = 4 leads to six different R_{χ} types:

⁴²² Detailed study [16] reveals that nevertheless an arbitrary DU(4) matrix can ⁴²³ be decomposed into a string of permutation matrices, a^{-1} matrices, and b^{-1} ⁴²⁴ matrices, where a^{-1} is a controlled square root of NOT and b^{-1} is a controlled ⁴²⁵ phase gate, e.g.

$$a^{26} \qquad a^{-1} = \frac{1}{2} \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1+i & 1-i \\ 0 & 0 & 1-i & 1+i \end{pmatrix} \quad \text{and} \quad b^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

However, for a given 4×4 matrix, in order to lower its level from χ^q to χ^{q-1} , it may be necessary to apply the 3-step procedure of Sect. 6 not just once but once, twice, or three times^b. To further lower the level (from χ^{q-1} to χ^{q-2} , χ^{q-3} , ...), the 3-step procedure needs to be applied, each time, either once or twice. As a result, the number of a^{-1} factors in the decomposition is 2q + 1 at most. One of the underlying reasons why a procedure similar to the DU(3) procedure is applicable, is the fact that all six matrix types (10) consist of 2×2 blocks, either equal to

$$\left(\begin{array}{cc} 0 & 0 \\ 0 & 0 \end{array}\right) \quad \text{or equal to} \quad \left(\begin{array}{cc} 1 & 1 \\ 1 & 1 \end{array}\right),$$

⁴²⁷ such that Appendix D can again be applied [16].

9. The Subgroup XDU(4)

The members of DU(4) where all eight line sums are equal to 1, form the 429 infinite subgroup XDU(4) of DU(4). The XDU(4) matrices of level 1 form 430 the subgroup P(4) of the 4! = 24 permutation matrices. This subgroup P(4)431 divides the supergroup XDU(4) into double cosets. E.g., there are eleven 432 double cosets of level 2, i.e. two of level 1 + i plus nine of level $(1 + i)^2$, 433 comprising a total of 2,472 matrices. Numbers for higher levels are given in 434 Table 2. The table suggests that the number of matrices grows like 225×4^q , 435 for q > 3. 436

An arbitrary member of XDU(4) can be factorized without phase gates.
Because the permutation group P(4) can be generated by two generators,
e.g.

$$\left(\begin{array}{rrrrr} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{array}\right) \quad \text{and} \quad \left(\begin{array}{rrrr} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{array}\right),$$

441 and because

428

440

442
$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} = (a^{-1})^2,$$

we may conclude that the group XDU(4) can be generated by two generators,

^bOnce if the R_{χ} type (10) contains a zero row or column; twice if the R_{χ} type contains zero entries but neither a zero row nor a zero column; either twice or three times if the R_{χ} type contains no zero entries.

444 e.g.

447

462

$${}_{445} \qquad g_1 \ = \ \frac{1}{2} \left(\begin{array}{cccc} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1+i & 1-i \\ 0 & 0 & 1-i & 1+i \end{array} \right) \qquad \text{and} \qquad g_2 \ = \ \left(\begin{array}{cccc} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{array} \right).$$

446 Finally, because g_2 can be decomposed as



we can conclude that the whole group XDU(4) can be generated by three different controlled square roots of NOT:

$${}^{450} \qquad \qquad \frac{1}{2} \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1+i & 1-i \\ 0 & 0 & 1-i & 1+i \end{pmatrix}, \qquad \frac{1}{2} \begin{pmatrix} 1+i & 1-i & 0 & 0 \\ 1-i & 1+i & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix},$$

Two of them control a same qubit, the third controls the other qubit. Two of them are controlled by a signal of same polarity, the remaining one is controlled by a signal of opposite polarity. We note that the first and third generator together generate a subgroup of XDU(4) isomorphic to XDU(3), i.e. all 4×4 matrices of the form

$$(\begin{array}{cc}1&\mathbb{O}\\\mathbb{O}&y\end{array}),$$

where \mathbb{O} denotes either the 1 × 3 zero matrix or the 3 × 1 zero matrix, and y is a member of XDU(3).

We summarize the present section by concluding that any matrix in XDU(4) can be written as a product of controlled square roots of NOT.

10. The Group DU(m), with m > 4

Each DU(m) matrix of level 1 consists of lines of the form [X, 0, 0, ..., 0](up to permutation of its vector components), where X is a number from $\{1, i, -1, -i\}$. There are $m! 4^m$ such matrices. They all are member of one of the m! subgroups of DU(m) isomorphic to DU(1)^m. We now consider a DU(m) matrix of level χ^1 . Because we have to guarantee the unit norm of each matrix line, a line can only exist (up to ordering) in two different forms: either [X, 0, 0, ..., 0] or [Y, Y, 0, 0, ..., 0], where Y is a number from $\{1/\chi, i/\chi, -1/\chi, -i/\chi\}$. Orthonormality implies that the matrix consists of merely

$$(X)$$
 and $\begin{pmatrix} Y & Y \\ Y & Y \end{pmatrix}$

⁴⁶⁷ blocks. As a result, there exist

468

$$m! 4^m \left[m! \sum_{k=0}^{\lfloor m/2 \rfloor} \frac{1}{k! (m-2k)!} - 1 \right]$$

such matrices. This amount can be written as $m! 4^m (\kappa_m - 1)$, where κ_m may 469 be expressed in terms of the confluent hypergeometric series ${}_{1}F_{1}(-j, k/2, -l/4)$, 470 which in turn can be expressed in terms of the Gamma function and the La-471 guerre polynomials. Additionally, κ_m is a number sequenced by Sloane [19] 472 and applied e.g. by Khruzin [20] and Proctor [21]. All these $m! 4^m (\kappa_m -$ 473 1) matrices belong to one of the subgroups of DU(m) isomorphic to some 474 group $\mathrm{DU}(2)^k \times \mathrm{DU}(1)^{m-2k}$ (with $0 \leq k \leq \lfloor m/2 \rfloor$). The number of these subgroups amounts to m! $(\lambda_m/2^m - 1)$, where the number λ_m is another 475 476 hypergeometric series (also expressable in terms of the Gamma function and 477 Laguerre polynomials) as well as another integer sequence [22]. Taking into 478 account the asymptotic behaviour [23] of the Laguerre polynomials for large 479 degree into account, as well as Stirling's formula, we find for $m \gg 1$: 480

481
$$\kappa_m \approx \frac{1}{\sqrt{2}} (m-1)^{m/2} \exp\left[-\frac{m}{2} + \frac{\sqrt{2m+1}}{2} + \frac{3}{8}\right]$$

482 $\lambda_m \approx \frac{1}{\sqrt{2}} (m-1)^{m/2} \exp\left[-\frac{m}{2} + \sqrt{2m+1}\right].$

The set of DU(m) matrices of level χ^2 is much richer, as they do also display lines of the form [Y, Z, Z, 0, 0, ..., 0] and [Z, Z, Z, Z, 0, 0, ..., 0], where Z is one of the complex numbers $\{\pm 1/2, \pm i/2\}$. such that, besides the single 1×1 block type, the single 2×2 block type, and the single 3×3 block type, i.e.

$$(X), \begin{pmatrix} Y & Y \\ Y & Y \end{pmatrix}, \text{ and } \begin{pmatrix} Y & Z & Z \\ Y & Z & Z \\ 0 & Y & Y \end{pmatrix},$$

489 they also may display five different 4×4 block types:

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etcetera. Results by Severini and Szöllősi [24] on unitary (though not necessarily dyadic) matrices demonstrate how the number of different $k \times k$ block types increases fast with increasing k.

We recall here some results of Sects. 4, 5, 6, and 8. For m = 1, we have only one level (i.e. level 1) with only one R_{χ} remainder class, i.e. the 1×1 matrix (1). For m = 2, we have only two levels: level 1 with only one remainder class, i.e.

$$\left(\begin{array}{cc}1&0\\0&1\end{array}\right),$$

and level χ with only one remainder class, i.e.

$$\left(\begin{array}{rr}1 & 1\\ 1 & 1\end{array}\right).$$

For m = 3, we have \aleph_0 levels: level 1 with only one remainder class, i.e.

$$\left(\begin{array}{rrr} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{array}\right),$$

and levels χ^q (with q > 0) with only one remainder class, i.e.

$$\left(\begin{array}{rrr} 0 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{array}\right).$$

For m = 4, we have \aleph_0 levels: level 1 with only one remainder class, i.e.

$$\left(\begin{array}{rrrrr} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{array}\right),$$

level χ with two remainder classes, i.e.

and levels χ^q (with q > 1) with six remainder classes, i.e. the classes (10).

20

We now conjecture that also in the case of arbitrary dimension m and arbitrary level (higher than χ^0), the R_{χ} types consist exclusively of 2 × 2 blocks

$$\left(\begin{array}{cc} 0 & 0\\ 0 & 0 \end{array}\right),$$
$$\left(\begin{array}{cc} 1 & 1\\ 1 & 1 \end{array}\right),$$

and (in case m is odd) a zero row and a zero column. We checked that this hypothesis is true for all matrices with m < 7. If the conjecture is generally true, then Appendix D may be applied once again, the role of the building blocks a^{-1} and b^{-1} being played by

500
$$a^{-1} = \frac{1}{2} \begin{pmatrix} 2 \cdot 1 & \mathbb{O} & \mathbb{O} \\ \mathbb{O} & 1+i & 1-i \\ \mathbb{O} & 1-i & 1+i \end{pmatrix}$$
 and $b^{-1} = \begin{pmatrix} 1 & \mathbb{O} & \mathbb{O} \\ \mathbb{O} & i & 0 \\ \mathbb{O} & 0 & 1 \end{pmatrix}$,

where $2 \cdot 1$ denotes twice the $(m-2) \times (m-2)$ unit matrix 1 and where ⁵⁰² \mathbb{O} denotes either the $(m-2) \times 1$ zero matrix or the $1 \times (m-2)$ zero ma-⁵⁰³ trix. For more details, the reader is referred to [16]. The procedure results ⁵⁰⁴ in a decomposition of an arbitrary DU(m) matrix into a finite number of ⁵⁰⁵ exclusively controlled square root of NOT gates, controlled phase gates and ⁵⁰⁶ classical reversible gates.

We close the present section by drawing attention to matrices of one particular level. Apart from zero, the smallest norm a unitary dyadic matrix entry can have, is $1/2^q$. If, in a line, all *m* entries have this minimum non-zero norm, then

$$m \frac{1}{2q} = 1$$

 2×2 blocks

512 Therefore, we define the critical number Q:

513
$$Q(m) = \log_2(m)$$
.

All matrices with q < Q have, in each row and in each column, at least one 514 zero. In fact, in each line, they have at least $m - 2^q = 2^Q - 2^q$ and at most 515 $m-1 = 2^{Q} - 1$ zeroes. Only matrices with $q \ge Q$ may have all entries 516 non-zero. In particular, if Q happens to be an integer, then matrices may 517 be of the Hadamard style, iff q = Q. The condition that Q is an integer, is 518 equivalent to m being of the form 2^w . All matrices representing a quantum 519 circuit (acting on w qubits) fulfil this condition. Therefore we investigate 520 this case in particular. 521

In case $m = 2^w$, matrices with q = Q = w may be of the Hadamard style [5, 18]. These $2^w \times 2^w$ matrices look like

524
$$\frac{1}{\chi^w} \begin{pmatrix} 1 & 1 & \dots & 1 \\ 1 & & & \\ \vdots & & & \\ 1 & & & \end{pmatrix},$$

i.e. χ^{-w} times a tensor product $F_2 \otimes F_2 \otimes \ldots \otimes F_2 \otimes F_4 \otimes F_4 \otimes \ldots \otimes F_4$ of Fourier transforms.

527 11. The Subgroup XDU(m), with m > 4

The number of XDU(m) matrices of level χ^0 is m!, whereas the number of XDU(m) matrices of level χ^1 is given by

530
$$m!(\mu_m - 1)$$

where μ_m is given either by the appropriate ${}_1F_1(-j, k/2, -l/4)$ series or by the appropriate Sloane sequence [25]. For $m \gg 1$, we have

533
$$\mu_m \approx \frac{1}{\sqrt{2}} (m-1)^{m/2} \exp\left[-\frac{m}{2} + \frac{\sqrt{2m+1}}{\sqrt{2}} + \frac{1}{4}\right].$$

For an XDU(m) of arbitrary level χ^q , we conjecture a decomposition without b^{-1} phase matrices. If $m = 2^w$, then the a^{-1} building block is the controlled square root of NOT with w - 1 controlling lines.

12. Conclusion

We have introduced the dyadic unitary matrix groups DU(m). The matrix 538 entries consist of Gaussian rationals with denominator 2^p . We have investi-539 gated into detail the cases DU(1), DU(2), DU(3), and DU(4). Whereas DU(1)540 is isomorphic to the cyclic group Z_4 of order 4, the group DU(2) is a finite 541 group of order 96, and all groups DU(m) with $m \ge 3$ are (countably) infinite. 542 We propose a simple algorithm to decompose an arbitrary member of DU(3)543 into a product of DU(3) matrices with exclusively denominators 2^0 and 2^1 . 544 A similar, though somewhat more complicated, algorithm is introduced for 545 m > 3. In case m is a power of 2, say equals 2^w , such decomposition is useful 546 for the synthesis of a quantum computer acting on w qubits, by applying 547 merely building blocks known as 'controlled square roots of NOT'. 548

Appendix A

In this appendix we prove the following theorem: if a unitary $m \times m$ matrix 550 has m identical row sums, then that row sum is on the unit circle. 551

Let M be an $m \times m$ unitary matrix, where the m row sums are de-552 noted $\sigma_1, \sigma_2, \ldots, \sigma_m$. We compute 553

554
$$\sum_{k} \sigma_{k} \overline{\sigma_{k}} = \sum_{k} \left[\left(\sum_{l} M_{kl} \right) \left(\sum_{n} M_{kn} \right) \right]$$

555
$$= \sum \left[\left(\sum M_{kl} \right) \left(\sum \overline{M_{kn}} \right) \right]$$

 $= \sum_{k} \sum_{l} \sum_{n} M_{kl} \overline{M_{kn}}$ 556

$$= \sum_{k} \sum_{l} \left(\sum_{n \neq l} M_{kl} M_{kn} + M_{kl} M_{kl} \right)$$

$$= \sum_{l} \sum_{n \neq l} \sum_{k} M_{kl} \overline{M_{kn}} + \sum_{k} \sum_{l} M_{kl} \overline{M_{kl}}$$

559
$$= \sum_{l} \sum_{n \neq l} 0 + \sum_{k} 1$$

560
$$= 0 + \sum_{k} 1$$

560

561

If all σ_k are equal to σ , this yields $m\sigma \overline{\sigma} = m$ and thus $\sigma \overline{\sigma} = 1$. The matrix M 562 can thus be written as the product of a matrix M' with contant row sum 1 563 and a scalar σ that merely is a complex phase. 564

Analogously, if a unitary matrix has all identical column sums, then that 565 column sum is on the unit circle. 566

Finally, if a unitary matrix has all row sums equal (say, σ) and all column 567 sums equal (say, τ), then these two sums are equal. The proof is trivial: it 568 suffices to compute, in two different ways, the sum of all matrix elements, 569 $\sum_{j} \sum_{k} M_{jk} = \sum_{j} \sigma = m\sigma$ and $\sum_{k} \sum_{j} M_{jk} = \sum_{k} \tau = m\tau$. 570

Appendix B

An example of a dyadic unitary matrix with dimension m equal to 3 and 572 level equal to 2 is given by 573

574
$$y = \frac{1}{2} \begin{pmatrix} 1-i & 1 & i \\ 1+i & -i & 1 \\ 0 & 1+i & 1-i \end{pmatrix}.$$

549

Its three eigenvalues are 1, $\exp(i\theta_1)$, and $\exp(i\theta_2)$, with $\theta_1 = -\frac{\pi}{2} - \theta$ and $\theta_2 = -\frac{\pi}{2} + \theta$, where θ is $\operatorname{Arccos}(3/4) \approx 41^{\circ}24'35''$.

Because the only rational multiples of π with a rational cosine [26] are $0 = \operatorname{Arccos}(1), \pi/3 = \operatorname{Arccos}(1/2), \pi/2 = \operatorname{Arccos}(0), 2\pi/3 = \operatorname{Arccos}(-1/2),$ $\pi = \operatorname{Arccos}(-1), 5\pi/3 = \operatorname{arccos}(-1/2), 3\pi/2 = \operatorname{arccos}(0), \text{ and } 5\pi/3 = \operatorname{arccos}(1/2),$ $\cos(1/2), \text{ neither } \theta_1 \text{ nor } \theta_2 \text{ is a rational multiple of } \pi.$ Therefore, the power sequence $\{y, y^2, y^3, \ldots\}$ is not periodic. Therefore the sequence $\{\ldots, y^{-2}, y^{-1}, y^0, y^1, y^2, \ldots\}$ forms a countably infinite group. As it is a cyclic subgroup of DU(3), this proves that DU(3) is at least countably infinite.

As an immediate consequence, DU(m) with m larger than 3 also is infinite. Suffice it to note that the $m \times m$ square matrix

$$\left(\begin{array}{cc} 1\!\!1 & \mathbb{O} \\ \mathbb{O} & y \end{array}\right),$$

where 1 represents the $(m-3) \times (m-3)$ unit matrix and \mathbb{O} either the $(m-3) \times 3$ zero matrix or the $3 \times (m-3)$ zero matrix, is a member of DU(m)and has infinite order.

Appendix C

591 C.1 Number of XDU(3) matrices

We assume six arbitrary integers a_1 , a_2 , a_3 , b_1 , b_2 , and b_3 (not all zero). With their help, we construct the following three vectors:

594
$$V_1 = \frac{1}{\chi^{q+1}} \Big[(a_1 - b_1) + i(a_1 + b_1) \quad (a_2 - b_2) + i(a_2 + b_2) \quad (a_3 - b_3) + i(a_3 + b_3) \Big]$$

595
$$V_2 = \frac{1}{\chi^{q+1}} \Big[(a_2 - b_2) + i(a_3 + b_3) \quad (a_3 - b_3) + i(a_1 + b_1) \quad (a_1 - b_1) + i(a_2 + b_2) \Big]$$

596
$$V_3 = \frac{1}{\chi^{q+1}} \Big[(a_3 - b_3) + i(a_2 + b_2) \quad (a_1 - b_1) + i(a_3 + b_3) \quad (a_2 - b_2) + i(a_1 + b_1) \Big].$$

^{χ^{q+1}} [^{χ^{q+1} [^{χ^{q+1} [^{χ^{q+1}} [^{χ^{q+1} [^{χ^{q+1} [^{χ^{q+1}} [^{χ^{q+1} [^{$\chi^{q+}}}}}}</sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup></sup>$

⁵⁹⁷ The numbers $(a_1-b_1)+i(a_1+b_1)$, $(a_2-b_2)+i(a_2+b_2)$, and $(a_3-b_3)+i(a_3+b_3)$ are divisible by 1+i,

599
$$(a_1 - b_1) + i(a_1 + b_1) = (a_1 + ib_1)(1 + i)$$
 etc.

Thus the vector V_1 is of level χ^q at most. We assume that the vector V_1 has exactly level χ^q , i.e. that at least one of the three numbers $a_1 + ib_1$, $a_2 + ib_2$, and $a_3 + ib_3$ is not divisible by χ . Detailed analysis [17] then demonstrates that the vectors V_2 and V_3 are not divisible by χ and thus have level χ^{q+1} . The three vectors V_1 , V_2 , and V_3 all have the same line sum,

605
$$\frac{1}{\chi^{q+1}} \left[\left(a_1 + a_2 + a_3 - b_1 - b_2 - b_3 \right) + i \left(a_1 + a_2 + a_3 + b_1 + b_2 + b_3 \right) \right]$$

The Group of Dyadic Unitary Matrices

$$= \frac{1}{\chi^{q+1}} (1+i) [(a_1+a_2+a_3)+i(b_1+b_2+b_3)]$$

$$= \frac{1}{\chi^q} [(a_1 + a_2 + a_3) + i(b_1 + b_2 + b_3)].$$

⁶⁰⁸ They also have the same norm,

$$\frac{1}{2^{q+1}} \left(2a_1^2 + 2b_1^2 + 2a_2^2 + 2b_2^2 + 2a_3^2 + 2b_3^2 \right)$$
$$= \frac{1}{2^q} \left(a_1^2 + a_2^2 + a_3^2 + b_1^2 + b_2^2 + b_3^2 \right).$$

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We assume that this norm is equal to 1,

612
$$(a_1^2 + a_2^2 + a_3^2 + b_1^2 + b_2^2 + b_3^2) / 2^q = 1.$$

⁶¹³ We also assume that the line sum equals 1. Therefore the norm of the line ⁶¹⁴ sum is equal to 1,

$$\left[(a_1 + a_2 + a_3)^2 + (b_1 + b_2 + b_3)^2 \right] / 2^q = 1$$

Subtracting the former result from the latter result yields that $a_1a_2 + a_2a_3 +$ 616 $a_3a_1+b_1b_2+b_2b_3+b_3b_1$ equals zero. Because straightforward calculation of the 617 inner product $V_1 \overline{V_2}$ leads to the value $(a_1 a_2 + a_2 a_3 + a_3 a_1 + b_1 b_2 + b_2 b_3 + b_3 b_1)/2^q$, 618 we can conclude that V_1 and V_2 are orthogonal to each other. Similarly, we 619 find that all three vectors V_1 , V_2 , and V_3 are orthogonal to one another. Thus 620 the triple $\{V_1, V_2, V_3\}$ gives rise to an XDU(3) matrix of level χ^{q+1} . In fact, 621 because of permutation of matrix lines, it actually gives rise to six different 622 XDU(3) matrices of level χ^{q+1} . 623

We now consider different triples $\{V_1, V_2, V_3\}, \{V'_1, V'_2, V'_3\}, \{V''_1, V''_2, V''_3\}, \{V''_1, V''_2, V''_3\}$ 624 ..., where V_1, V'_1, V''_1, \ldots all are vectors of level χ^q . Then V_1 is orthogonal 625 to V_2 and V_3 , but not to V'_2 , V''_3 , V''_2 , V''_3 , V''_2 , ... [17]. Thus only the triples 626 $\{V_1, V_2, V_3\}, \{V'_1, V'_2, V'_3\}, \dots$ can give rise to an XDU(3) matrix of level χ^{q+1} . 627 As each such triple gives rise to six XDU(3) matrices, for any $q \ge 0$, there 628 are 6 times as many XDU(3) matrices of level χ^{q+1} as there are vectors of 629 level χ^q . Because with each vector V_1 of level χ^q correspond two vectors (V_2 630 and V_3) of level χ^{q+1} , the number of vectors with a same level χ^q increases 631 like 2^{q} . Therefore, the number of matrices similarly increases as 2^{q} and thus 632 equals $c \times 2^q$, with c some appropriate constant. The coefficient c is identified 633 by remarking that there are eighteen XDU(3) matrices of level χ^1 (Table 2). 634 One thus finds c = 9. We conclude: for any $q \ge 1$, there exist 9×2^q XDU(3) 635 matrices of level χ^q . 636

$_{637}$ C.2 Number of DU(3) matrices

⁶³⁸ A similar reasoning as in Subappendix C.1 exists for the DU(3) matrices [17]. ⁶³⁹ Again we assume vectors V_1, V'_1, V''_1, \ldots of level χ^q . With each vector V_1

| $\begin{array}{c} R_2(g) = \\ G_j \end{array}$ | $R_2(g a) = G_j R_2(a)$ | $R_2(g b a) = \\G_j R_2(b a)$ | | |
|--|--|--|--|--|
| $\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \\ \begin{pmatrix} 1 & 1 \\ i & i \end{pmatrix} \\ \begin{pmatrix} 1 & i \\ 1 & i \end{pmatrix} \\ \begin{pmatrix} 1 & i \\ 1 & i \end{pmatrix} \\ \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \\ \begin{pmatrix} i & i \\ i & i \end{pmatrix}$ | $\begin{pmatrix} 1+i & 1+i \\ 1+i & 1+i \end{pmatrix}$ $\begin{pmatrix} 1+i & 1+i \\ 1+i & 1+i \end{pmatrix}$ $\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$ $\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$ $\begin{pmatrix} 1+i & 1+i \\ 1+i & 1+i \end{pmatrix}$ | $\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \\ \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \\ \begin{pmatrix} 1+i & 1+i \\ 1+i & 1+i \end{pmatrix} \\ \begin{pmatrix} 1+i & 1+i \\ 1+i & 1+i \end{pmatrix} \\ \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$ | | |

Table 3: The five R_2 remainder matrices G_j .

of level χ^q now correspond four vectors $(V_2, V_3, V_4, \text{ and } V_5)$ of level χ^{q+1} , 640 such that the number of vectors with a same level χ^q grows like 4^q . With 641 each quintuple $\{V_1, V_2, V_3, V_4, V_5\}$ correspond two triples, i.e. $\{V_1, V_2, V_3\}$ and 642 $\{V_1, V_4, V_5\}$ and therefore twice six matrices of DU(3). The number of ma-643 trices grows like the number of vectors, i.e. equals $c \times 4^{q}$. We identify the 644 coefficient c by remarking that there are 2,304 DU(3) matrices of level χ^1 645 (Table 1). One thus finds c = 576. We conclude: for any $q \ge 1$, there exist 646 576×4^q DU(3) matrices of level χ^q . 647

Appendix D

Applying Gaussian primes to Sect. 5 leads to the conclusion that the group DU(2) consists of 32 matrices of level 1 and 64 matrices g of level χ . The latter all have the same remainder matrix $R_{\chi}(g)$ equal to

$$\left(\begin{array}{rr}1 & 1\\ 1 & 1\end{array}\right),$$

⁶⁴⁹ but can have five and only five different remainder matrices $R_2(g)$ (up to ⁶⁵⁰ equivalence by row or column swapping). We call these 2 × 2 matrices ⁶⁵¹ G_1, G_2, \ldots , and G_5 , respectively, see Table 3.

We now introduce two particular DU(2) matrices: a of level χ and b of level 1,

$$a = \frac{1}{\chi} \begin{pmatrix} -i & 1\\ 1 & -i \end{pmatrix}$$
 and $b = \begin{pmatrix} -i & 0\\ 0 & 1 \end{pmatrix}$

We compute the matrices $R_2(ga) = G_j R_2(a)$ and $R_2(gba) = G_j R_2(ba)$. With

$$R_2(a) = \begin{pmatrix} i & 1 \\ 1 & i \end{pmatrix}$$
 and $R_2(ba) = \begin{pmatrix} 1 & i \\ 1 & i \end{pmatrix}$,

this yields Table 3. We see that in two cases multiplication by $R_2(a)$ leads to the 2 × 2 zero matrix and that in the remaining three cases multiplication by $R_2(ba)$ leads to the zero matrix. A zero $R_2(g)R_2(a)$ matrix reveals that the product ga is not of level χ^2 but instead of level 1, whereas a zero $R_2(g)R_2(ba)$ matrix reveals that the product gba is of level 1. We thus may conclude that each of the sixty-four DU(2) matrices g of level χ can be lowered to level 1 either through multiplication by a or through multiplication by ba.

⁶⁶² Only 2 of the 64 matrices g belong to XDU(2). They both lead to type ⁶⁶³ G_4 , such that $R_2(ga)$ is the zero matrix.

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