A Birkhoff connection between quantum circuits and linear classical reversible circuits

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Abstract. Birkhoff's theorem tells how any doubly stochastic matrix can be decomposed as a weighted sum of permutation matrices. Similar theorems on unitary matrices reveal a connection between quantum circuits and linear classical reversible circuits. It triggers the question whether a quantum computer can be regarded as a superposition of classical reversible computers.

1 Introduction

Let D be an arbitrary $n \times n$ doubly stochastic matrix. This means that all entries D_{jk} are real and satisfy $0 \leq D_{jk} \leq 1$ and that all line sums (i.e. the n row sums and the n column sums) are equal to 1. Let $\mathrm{P}(n)$ be the group of $n \times n$ permutation matrices. Birkhoff [1] has demonstrated

Theorem 1 *Any $n \times n$ doubly stochastic matrix D can be written*

$$D = \sum_j c_j P_j$$

with all $P_j \in P(n)$ and the weights c_j real, satisfying both $0 \leq c_j \leq 1$ and $\sum_j c_j = 1$.

Because unitary matrices describe quantum circuits [2] and permutation matrices describe classical reversible circuits [3], the question arises whether a similar theorem holds for matrices from the unitary group $\mathrm{U}(n)$. In a sloppy way, one might reformulate the question as:

> **Is a quantum computer a quantum superposition of a finite number of classical (reversible) computers?**

It is a surprise that (to our knowledge) this problem has not been discussed in the literature.

It is clear that a simple positive answer to the above question is not possible. Indeed, any sum $\sum_j c_j P_j$ is a matrix with identical line sums (equal to $\sum_j c_j$), whereas an arbitrary unitary matrix usually does not have identical line sums. Moreover, if all c_j are real, then the matrix $\sum_j c_j P_j$ has exclusively real entries, again a property not shown by an arbitrary unitary matrix. Nevertheless, below we will present some Birkhoff-like theorems concerning $n \times n$ unitary matrices in general and $2^w \times 2^w$ unitary matrices in peculiar.

2 The ZXZ decomposition of a unitary matrix

Each quantum circuit acting on w qubits is represented by a $2^w \times 2^w$ unitary matrix. Such matrix thus is a member of the unitary group $\mathrm{U}(n)$ with $n = 2^w$. In light of quantum circuit decomposition, the (sub)group structure of $\mathrm{U}(n)$ is particularly important. We note the following two useful subgroups [4] [5]:

- $\mathrm{XU}(n)$, i.e. the group of $\mathrm{U}(n)$ matrices with all line sums equal to 1 and
- $\mathrm{ZU}(n)$, i.e. the group of diagonal $\mathrm{U}(n)$ matrices with upper-left entry equal to 1.

Whereas $\mathrm{U}(n)$ is a group of dimension n^2, $\mathrm{XU}(n)$ is a group of dimension $(n-1)^2$ and $\mathrm{ZU}(n)$ is a group of dimension $n-1$.

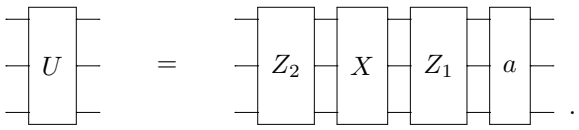
Idel and Wolf [6] proved the following theorem:

Theorem 2 *Every $n \times n$ unitary matrix U can be decomposed as*

$$U = a\, Z_1 X Z_2 \ , \tag{1}$$

where both Z_1 and Z_2 are ZU(n) matrices, where X is an XU(n) matrix, and a is a unit-modulus scalar.

Proof of the theorem is based on simplectic topology and, unfortunately, is not constructive. There exists an iterative method [7] for, given a matrix U, finding a set (a, Z_1, X, Z_2) with arbitrary numerical precision. If n equals 2^w, then the matrix decomposition expresses the decomposition of a quantum circuit acting on w qubits [8]. The 3-qubit case ($n = 8$) looks like



3 The Birkhoff decomposition of the XU matrix

De Baerdemacker et al. [9] proved the following theorem:

Theorem 3 *Every XU(n) matrix X can be decomposed as*

$$X = \sum_{j=1}^{n!} c_j P_j \ ,$$

where P_j are the $n \times n$ permutation matrices and c_j are complex numbers, such that both $\sum c_j = 1$ and $\sum |c_j|^2 = 1$.

De Baerdemacker et al. provide an algorithm to find any possible set of appropriate weights c_j. This set is far from unique (except if $n = 2$).

De Vos and De Baerdemacker [10] [11] demonstrated, in case n equals a power of 2 (say, $n = 2^w$), the following theorem:

Theorem 4 *Every XU(2^w) matrix X can be decomposed as*

$$X = \sum_{j=1}^{N(w)} c_j E_j \ ,$$

where j runs over all $2^w \times 2^w$ epicirculant permutation matrices E_j, where c_j are complex numbers, such that both $\sum c_j = 1$ and $\sum |c_j|^2 = 1$, and $N(w)$ equals $2^w(2^w - 1)(2^w - 2)(2^w - 2^2)...(2^w - 2^{w-1})$.

In next section will be explained what is meant with 'epicirculant matrix'. Theorem 4 is stronger than Theorem 3, because $N(w)$ scales much better than $(2^w)!$ for large w, as can be seen in the table:

w	2^w	$(2^w)!$	$N(w)$
1	2	2	2
2	4	24	24
3	8	40,320	1,344
4	16	20,922,789,888,000	322,560

One possible set of weights c_j is given by

$$c_j = \delta_{1,j} + \frac{2^w - 1}{N(w)} \ \left[\ \mathrm{Trace}\left(E_j^{-1} X\right) - \mathrm{Trace}\left(E_j\right) \ \right] \ ,$$

where the Kronecker delta assumes that the epicirculant matrix E_1 is the $2^w \times 2^w$ unit matrix.

4 Epicirculant matrices

Before giving the definition of a $2^w \times 2^w$ epicirculant matrix, it is useful to introduce some convenient conventions:

Remark 1 *In the present paper, rows and columns of any $2^w \times 2^w$ matrix are numbered from 0 to $2^w - 1$ (instead of the conventional numbering from 1 to 2^w) and each such number is represented by the $w \times 1$ matrix consisting of the w bits of the binary notation of the row-or-column number.*

E.g. the upper-left entry of the 8×8 matrix A is entry $A_{0,0} = A_{(0,0,0)^T,(0,0,0)^T}$, whereas its lower-right entry is denoted $A_{7,7} = A_{(1,1,1)^T,(1,1,1)^T}$. Further, we choose to order bits from least significant to most significant bit. E.g., for $w = 3$, the vector $(1, 1, 0)^T$ denotes the number 3.

Definition 1 *A $2^w \times 2^w$ epicirculant matrix M is a $2^w \times 2^w$ matrix, such that each entry $M_{j,k}$ equals the entry $M_{0,c}$ with $c = k - xj$, where the multiplication xj is a matrix multiplication performed modulo 2, and where x is some invertible $w \times w$ matrix with entries from $\{0, 1\}$, called the pitch matrix. The subtraction $k - xj$ is a vector addition performed modulo 2.*

E.g. the following matrix is an 8×8 epicirculant matrix with pitch matrix $x = \left(\begin{smallmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 1 \end{smallmatrix}\right)$:

$$\begin{pmatrix} m_0 & m_1 & m_2 & m_3 & m_4 & m_5 & m_6 & m_7 \\ m_1 & m_0 & m_3 & m_2 & m_5 & m_4 & m_7 & m_6 \\ m_4 & m_5 & m_6 & m_7 & m_0 & m_1 & m_2 & m_3 \\ m_5 & m_4 & m_7 & m_6 & m_1 & m_0 & m_3 & m_2 \\ m_6 & m_7 & m_4 & m_5 & m_2 & m_3 & m_0 & m_1 \\ m_7 & m_6 & m_5 & m_4 & m_3 & m_2 & m_1 & m_0 \\ m_2 & m_3 & m_0 & m_1 & m_6 & m_7 & m_4 & m_5 \\ m_3 & m_2 & m_1 & m_0 & m_7 & m_6 & m_5 & m_4 \end{pmatrix} . \tag{2}$$

Thanks to the fact that matrix x is invertible, not only each of the eight rows but also each of the eight columns contains exactly one m_0, one m_1, ..., and one m_7. If all entries of its upper row (i.e. row 0) are equal to 0, except one entry equal to 1 (in column s), then an epicirculant matrix is an epicirculant permutation matrix. The vector representing position s is called the shift vector. There exist as many different epicirculant permutation matrices as there exist possible shift vectors (i.e. 2^w) times the number of possible pitch matrices (i.e. $(2^w - 1)(2^w - 2)(2^w - 2^2)...(2^w - 2^{w-1})$). Because

- the shift vectors form a group isomorphic to the direct product $(\mathbf{C}_2)^w$ of w cyclic groups, each of order 2, and therefore of order 2^w and
- the pitch matrices form a group isomorphic to the general linear group GL(w,2) of order $(2^w - 1)(2^w - 2)(2^w - 2^2)...(2^w - 2^{w-1})$,

the epicirculant permutation matrices form a group [12] isomorphic to the general affine group GA(w,2) of order $N(w)$, isomorphic to the semidirect product $(\mathbf{C}_2)^w$ **:** GL(w,2). E.g. the following matrix is an 8×8 epicirculant permutation

matrix with shift vector $s = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ and pitch matrix $x = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}$:

$$\begin{pmatrix} 0&0&1&0&0&0&0&0 \\ 0&0&0&1&0&0&0&0 \\ 0&0&0&0&0&0&1&0 \\ 0&0&0&0&0&0&0&1 \\ 0&0&0&0&1&0&0&0 \\ 0&0&0&0&0&1&0&0 \\ 1&0&0&0&0&0&0&0 \\ 0&1&0&0&0&0&0&0 \end{pmatrix} . \tag{3}$$

It is obtained from matrix (2) by choosing $m_2 = 1$ and $m_k = 0$ for $k \neq 2$. We note that, if s is the $w \times 1$ zero matrix and x is the $w \times w$ unit matrix, then the corresponding epicirculant permutation matrix is the $2^w \times 2^w$ unit matrix E_1.

We have [11]:

Lemma 1 *Each epicirculant permutation matrix E can be written as the product of a zero-shift epicirculant permutation matrix L and a unit-pitch epicirculant permutation matrix N:*

$$E = LN \ .$$

E.g. matrix (3) has the decomposition

$$\begin{pmatrix} 1&0&0&0&0&0&0&0 \\ 0&1&0&0&0&0&0&0 \\ 0&0&0&0&1&0&0&0 \\ 0&0&0&0&0&1&0&0 \\ 0&0&0&0&0&0&1&0 \\ 0&0&0&0&0&0&0&1 \\ 0&0&1&0&0&0&0&0 \\ 0&0&0&1&0&0&0&0 \end{pmatrix} \begin{pmatrix} 0&0&1&0&0&0&0&0 \\ 0&0&0&1&0&0&0&0 \\ 1&0&0&0&0&0&0&0 \\ 0&1&0&0&0&0&0&0 \\ 0&0&0&0&0&0&1&0 \\ 0&0&0&0&0&0&0&1 \\ 0&0&0&0&1&0&0&0 \\ 0&0&0&0&0&1&0&0 \end{pmatrix} . \tag{4}$$

The left matrix has shift equal to $\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$ and pitch equal to $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}$, whereas the right matrix has shift vector $\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ and pitch matrix $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$.

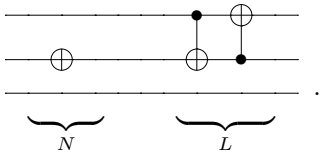
From classical reversible computation [3] [13] [14] [15], we know the following two lemmas:

Lemma 2 *An arbitrary zero-shift epicirculant permutation matrix L represents a linear circuit, i.e. a circuit consisting exclusively of singly controlled* `NOT` *gates (a.k.a.* `FEYNMAN` *gates).*

and

Lemma 3 *An arbitrary unit-pitch epicirculant permutation matrix N represents a circuit consisting merely of a stack of w single-qubit gates, each either an* `IDENTITY` *gate or a* `NOT` *gate. We call such stack a* `NOT` *stack.*

E.g. the product (4) represents the circuit cascade



In general, N consists of 0 to w NOTs and L consists of $\mathcal{O}(w^2)$ or $\mathcal{O}(\frac{w^2}{\log(w)})$ controlled NOTs, depending on the synthesis method applied [13] [14].

5 The Birkhoff decomposition of the two ZU matrices

Because a member Z of the group ZU(n) is diagonal, it cannot be decomposed as a weighted sum $\sum c_j P_j$ of permutation matrices P_j, such that the weight sum $\sum c_j$ equals 1. Indeed, if $\sum c_j = 1$, then all line sums of the matrix $\sum c_j P_j$ are equal to 1. Except for the $n \times n$ unit matrix, no diagonal matrix has this property. For this reason, we decompose the matrices Z_1 and Z_2 of (1) according to

$$Z_1 = GX_1G^{-1} \quad \text{and} \quad Z_2 = GX_2G^{-1} \ , \tag{5}$$

where G is a constant $n \times n$ (dephased) Hadamard matrix [16]. As the unitary matrices Z_1 and Z_2 have unit upper-left entry, automatically, X_1 and X_2 (equal to $G^{-1}Z_1G$ and $G^{-1}Z_2G$, respectively) have all line sums equal to 1.

If $n = 2^w$, we choose the following Hadamard matrix:

$$G = H \otimes H \otimes ... \otimes H \ , \tag{6}$$

i.e. the Kronecker product of w small (i.e. 2×2) Hadamard matrices

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \ . \tag{7}$$

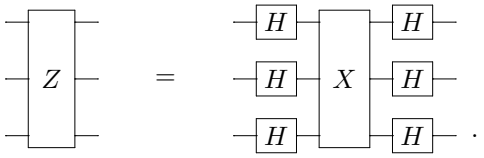
The matrix G has following entries:

$$G_{a,b} = \frac{1}{\sqrt{2^w}} \ (-1)^{f(a,b)} \ ,$$

where $f(x, y)$ is the sum of the bitwise product of the binary numbers x and y and hence the matrix product of the row vector x^T and the column vector y:

$$f(x, y) = \sum_j x_j y_j \bmod 2 = x^T y \ .$$

With this choice of G, the two matrix decompositions (5) represent the following circuit decomposition:



As the unitary matrices Z_1 and Z_2 are diagonal, automatically, X_1 and X_2 are epicirculant with unit pitch matrix. Indeed, if a $2^w \times 2^w$ matrix D is diagonal and G is given by (6-7), then an arbitrary entry of the product $G^{-1}DG$ is given by

$$\begin{aligned}(G^{-1}DG)_{j,k} &= \sum_r \sum_s (G^{-1})_{j,r} D_{r,s} G_{s,k} \\ &= \sum_r \frac{1}{\sqrt{2^w}} \, (-1)^{r^T j} D_{r,r} \, \frac{1}{\sqrt{2^w}} \, (-1)^{r^T k} \\ &= \frac{1}{2^w} \, \sum_r (-1)^{r^T (k-j)} \, D_{r,r} \ .\end{aligned}$$

We note that $(G^{-1}DG)_{0,k-j} = \frac{1}{2^w} \, \sum_r (-1)^{r^T (k-j)} \, D_{r,r}$ equals $(G^{-1}DG)_{j,k}$, which means that $G^{-1}DG$ is epicirculant according to Definition 1 with x equal to the $w \times w$ unit matrix.

Any $2^w \times 2^w$ epicirculant matrix M satisfies

$$M = \sum_{m=0}^{2^w - 1} M_{0,m} \, F_m \ ,$$

with F_m the epicirculant permutation matrix with shift vector equal to m and same pitch matrix as M. Hence, X_1 and X_2 satisfy the (short) Birkhoff sums:

$$X_1 = \sum_{j=1}^{2^w} a_j E_j \quad \text{and} \quad X_2 = \sum_{j=1}^{2^w} b_j E_j \ ,$$

where the E_j are the epicirculant permutation matrices with unit pitch matrix. Because X_1 and X_2 are unitary, we immediately have $\sum |a_j|^2 = \sum |(X_1)_{0,j}|^2 = 1$ and $\sum |b_j|^2 = \sum |(X_2)_{0,j}|^2 = 1$. Moreover, because both X_1 and X_2 have row sums equal to 1, we have $\sum a_j = \sum (X_1)_{0,j} = 1$ and $\sum b_j = \sum (X_2)_{0,j} = 1$.

The unit-pitch epicirculant permutation matrices form a group isomorphic to the direct product $(\mathbf{C}_2)^w$ of order 2^w. According to Lemma 3, such permutation matrix E_j represents a `NOT` stack.

6 The Birkhoff decomposition of the scalar factor

The unit-modulus scalar a in (1) is to be interpreted as a $2^w \times 2^w$ unitary matrix A, i.e. a times the $2^w \times 2^w$ unit matrix. It thus is also a times the $2^w \times 2^w$ identity permutation matrix. Therefore it is a weighted 'sum' of permutation matrices:

$$A = \sum_j d_j P_j = a P_1 \ .$$

We have $\sum |d_j|^2 = |a|^2 = 1$; however, the sum $\sum_j d_j = a$ usually is <u>not</u> equal to 1.

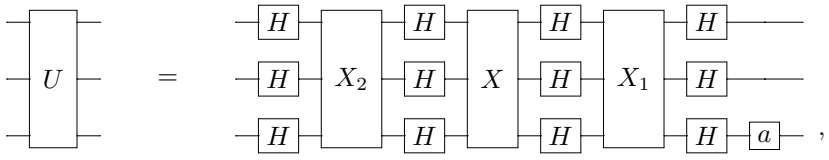
The matrix A equals the Kronecker product

$$I \otimes I \otimes I \otimes ... \otimes I \otimes \begin{pmatrix} a & 0 \\ 0 & a \end{pmatrix} \otimes I \otimes I \otimes I \otimes ... \otimes I \ ,$$

with $w-1$ appearances of the factor $I = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right)$ and, within the product, arbitrary position of the factor $\left(\begin{smallmatrix} a & 0 \\ 0 & a \end{smallmatrix}\right)$. The scalar a thus represents a w-qubit quantum circuit with merely one single-qubit gate acting on an arbitrary wire.

7 The Birkhoff decomposition of the U matrix

From the above discussion, we see that any w-qubit quantum circuit can be constructed as the following cascade:



containing

- $4w + 1$ single-qubit gates represented by U(2) matrices:
  - $4w$ `HADAMARD` gates and
  - one `PHASE-SHIFT` gate

  and
- three w-qubit circuits represented by XU(2^w) matrices:
  - one decomposable as a weighted sum of classical reversible circuits consisting of 2-bit gates (controlled `NOT` gates) and single-bit gates (`NOT` gates) and
  - two decomposable as a weighted sum of classical reversible circuits consisting exclusively of single-bit gates (`NOT` gates).

We have

$$\begin{aligned} U &= a\, Z_1 X Z_2 \\ &= a\, G X_1 G^{-1}\, X\, G X_2 G^{-1} \\ &= a\, G\,(\sum_{j_1=1}^{2^w} a_{j_1} E_{j_1})\, G^{-1}\,(\sum_{j=1}^{N(w)} c_j E_j)\, G\,(\sum_{j_2=1}^{2^w} b_{j_2} E_{j_2})\, G^{-1} \\ &= a \sum_{j_1=1}^{2^w} \sum_{j=1}^{N(w)} \sum_{j_2=1}^{2^w} a_{j_1} c_j b_{j_2}\, G E_{j_1} G^{-1} E_j G E_{j_2} G^{-1} \ . \end{aligned} \tag{8}$$

We note that the identities

and

imply that each of the two compositions $GE_{j_1}G^{-1}$ and $GE_{j_2}G^{-1}$ can be replaced by a stack of w gates, each either an `IDENTITY` gate, representing the unit matrix $\left(\begin{smallmatrix}1&0\\0&1\end{smallmatrix}\right)$, or a `Z` gate, representing the matrix

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

Thus:

Lemma 4 *A* `NOT` *stack sandwiched between two* `HADAMARD` *stacks is a* `Z` *stack.*

The `Z` stacks form a group isomorphic to $(\mathbf{C}_2)^w$ and are represented by diagonal $2^w \times 2^w$ matrices with an upper-left entry equal to 1 and all other diagonal entries equal to ± 1. Thus the matrix $GE_{j_1}G^{-1}E_jGE_{j_2}G^{-1}$ within eqn (8) represents an epicirculant permutation matrix sandwiched between two `Z` stacks and hence is a signed epicirculant permutation matrix. We summarise the present section by a new theorem:

Theorem 5 *Every U(2^w) matrix U can be decomposed as*

$$U = a \sum_{j=1}^{M(w)} c_j S_j \ ,$$

where a is a complex (unit-modulus) scalar, where j runs over $2^w \times 2^w$ signed epicirculant permutation matrices S_j, where c_j are complex numbers, such that both $\sum c_j = 1$ and $\sum |c_j|^2 = 1$, and $M(w)$ equals $4^w \times 2^w(2^w-1)(2^w-2)(2^w-2^2)...(2^w-2^{w-1})$.

8 Conclusion

We conclude that an arbitrary quantum computer can be regarded as a weighted sum of almost-classical reversible computers. Each of these reversible computers consists of two surprisingly simple classical parts:

- one linear circuit (composed of exclusively controlled `NOT`s) and
- one `NOT` stack

and three small quantum parts:

- one complex scalar and
- two `Z` stacks.

Whereas a matrix product represents a circuit cascade, a matrix sum does not represent a simple circuit structure. Recently, there have been some attempts [17] [18] to apply a weighted matrix sum for quantum circuit synthesis. However, this so-called 'reuse method' is only efficient (in terms of gate count and ancilla count) in very specific cases. Further research may reveal the full impact of the unitary Birkhoff theorems on quantum computation. Future work may lead to applications in simulation of quantum systems by means of classical computers.

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