Clifford Algebras, Spin Groups and Qubit Trees

Alexander Yurievich Vlasov

P. V. Ramzaev Research Institute of Radiation Hygiene, Saint Petersburg, Russia. E-mail: a.vlasov@niirg.ru

Editors: *Leonardo Chiatti* & *Danko D. Georgiev*

Article history: Submitted on September 1, 2022; Accepted on November 28, 2022; Published on December 1, 2022.

Representations of Spin groups and Clifford algebras derived from the structure of qubit trees are introduced in this work. For ternary trees the construction is more general and reduction to binary trees is formally defined by deletion of superfluous branches. The usual Jordan–Wigner construction also may be formally obtained in this approach by bringing the process up to trivial qubit chain (trunk). The methods can also be used for effective simulation of some quantum circuits corresponding to the binary tree structure. The modeling of more general qubit trees, as well as the relationship with the mapping used in the Bravyi–Kitaev transformation, are also briefly discussed.

Quanta 2022; 11: 97–114.

1 Introduction

In previous work [1] on effective modeling of quantum state transfer in qubit chains, the problem of generalizing the suggested approach to arbitrary graphs was raised. This present work provides an extension of some methods used for qubit chains in Ref. [1] to qubit trees together with appropriate applications. It is also interesting from the point of view of generalizing the Jordan–Wigner transformations [2] to trees and more general graphs discussed in other works [3–7].

The approach developed in this work associates representations of Clifford algebras and Spin group with ternary and binary qubit trees. It can be more naturally defined by ternary trees with transition to binary trees using some 'pruning'. The application of similar ternary trees for fermion-to-qubit mapping was also discussed recently in Ref. [8].

Some preliminaries about Clifford algebras and Spin groups with application to the construction of quantum gates are introduced in Section 2. Representations of Clifford algebras and Spin groups using ternary qubit trees and deterministic finite automata are defined in Section 3, together with the description of a 'pruning process' that produces new trees by deletion of the branches. The procedure can also be used for the construction of binary qubit trees, which are introduced in Section 4. The binary trees can be considered as more natural generalization of some methods touched upon earlier in Ref. [1] due to the possibility of using some supplementary tools such as annihilation and creation operators discussed in Section 5. The application of the binary qubit trees in the construction of effectively modeled quantum circuits is described in Section 6 with some examples appropriate for the theory of quantum computation and communication.

The different scheme of qubit encoding by so-called Fenwick trees was also discussed in Ref. [9] for possible application to the Bravyi–Kitaev transformation [10]. For trees of arbitrary size, the number of children for some qubit nodes may not be limited. Such models can be encoded by an alternative version of binary trees presented in Section 7.1 and an example of application to Bravyi–Kitaev encoding is given in Section 7.2.

2 Preliminaries

Let us recollect the standard properties and definitions for Clifford algebras and Spin groups [11, 12] that will be needed in the next sections. For the vector space $\mathbb{V} = \mathbb{F}^n$ (where $\mathbb{F}$ is $\mathbb{R}$ or $\mathbb{C}$) the Clifford algebra $\mathcal{Cl}(\mathbb{V})$ provides linear embedding of vector $\mathbf{v} \in \mathbb{V}$ with the property

$$\mathfrak{e}\colon \mathbb{V} \longrightarrow \mathcal{Cl}(\mathbb{V}), \quad (\mathfrak{e}(\mathbf{v}))^2 = -|\mathbf{v}|^2\mathbb{1}, \tag{1}$$

where $\mathbb{1}$ is the unit of the algebra and $|\mathbf{v}|$ is a norm of the vector. For a vector $\mathbf{v} \in \mathbb{V}$ with coordinates v_k, the embedding is written as

$$\mathbf{v} = (v_1, \ldots, v_n), \quad \mathfrak{e}(\mathbf{v}) = \sum_{k=1}^{n} v_k \mathfrak{e}_k, \tag{2}$$

where $\mathfrak{e}_k$ are *generators of Clifford algebra*. The possibility to work with complex vector spaces $\mathbb{V} = \mathbb{C}^n$ is desirable for many models below, but some definitions and examples may be more naturally introduced for the real case $\mathbb{V} = \mathbb{R}^n$. The Minkowski (pseudo-Euclidean) norm is not considered here and for the Euclidean case Eq. (1) can be rewritten using Eq. (2) as

$$\{\mathfrak{e}_j, \mathfrak{e}_k\} \doteq \mathfrak{e}_j\mathfrak{e}_k + \mathfrak{e}_k\mathfrak{e}_j = -2\delta_{jk}\mathbb{1}, \quad j, k = 1, \ldots, n. \tag{3}$$

Due to the relations given in Eq. (3), the maximal number of different products of generators up to sign is 2^n and Clifford algebra with such dimension is called *universal* and denoted further $\mathcal{C\ell}(n, \mathbb{F})$. The natural non-universal examples are the *algebra of Pauli matrices*

$$\hat{\sigma}^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}^y = \begin{pmatrix} 0 & -\imath \\ \imath & 0 \end{pmatrix}, \quad \hat{\sigma}^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{4}$$

for $\mathbb{V} = \mathbb{C}^3$ and the *algebra of quaternions* $\mathbb{H}$ for 3D real space $\mathbb{V} = \mathbb{R}^3$. The dimension of such algebras is not maximal and one generator in this case could be dropped to satisfy universality condition, but it may not be always justified due to the structure of a model.

For complex vector space with even dimension $\mathbb{C}^{2m}$ the universal Clifford algebra $\mathcal{C\ell}(2m, \mathbb{C})$ may be represented as $2^m \times 2^m$ complex matrix algebra [11]. The generators of $\mathcal{C\ell}(2m, \mathbb{C})$ can be expressed using the Jordan–Wigner [2] representation

$$\begin{aligned} \mathfrak{e}_{2k-1} &= \imath\, \underbrace{\hat{\sigma}^z \otimes \cdots \otimes \hat{\sigma}^z}_{k-1} \otimes \hat{\sigma}^x \otimes \underbrace{\mathbb{1} \otimes \cdots \otimes \mathbb{1}}_{m-k}, \\ \mathfrak{e}_{2k} &= \imath\, \underbrace{\hat{\sigma}^z \otimes \cdots \otimes \hat{\sigma}^z}_{k-1} \otimes \hat{\sigma}^y \otimes \underbrace{\mathbb{1} \otimes \cdots \otimes \mathbb{1}}_{m-k}, \end{aligned} \tag{5}$$

where $k = 1, \ldots, m$.

In odd dimensions, the universal Clifford algebra $\mathcal{C\ell}(2m+1, \mathbb{C})$ can be represented using block diagonal matrices

$$\begin{pmatrix} \mathbf{A} & \mathbf{0} \\ \mathbf{0} & \mathbf{B} \end{pmatrix} \in \mathcal{C\ell}(2m+1, \mathbb{C}), \quad \mathbf{A}, \mathbf{B} \in \mathcal{C\ell}(2m, \mathbb{C}), \tag{6}$$

i.e., as the direct sum of *two* $\mathcal{C\ell}(2m, \mathbb{C})$, but an irreducible representation with the half of maximal dimension also exists. It may be treated as $\mathcal{C\ell}(2m, \mathbb{C})$ with the additional generator that can be expressed up to possible imaginary unit multiplier as product of all $2m$ generators. For the representation given by Eq. (5), it may be written as

$$\mathfrak{e}_{2m+1} = \imath\, \underbrace{\hat{\sigma}^z \otimes \cdots \otimes \hat{\sigma}^z}_{m}\,. \tag{5$'$}$$

This case is essential for many examples considered below. Using $2m$ generators Eq. (5) together with the extra one Eq. (5′) denoted as $\mathfrak{e}_j^{(2m)}$, the representation of generators $\mathfrak{e}_j^{(2m+1)}$ respecting Eq. (6) for universal Clifford algebra $\mathcal{C\ell}(2m+1, \mathbb{C})$ can be written as

$$\mathfrak{e}_j^{(2m+1)} = \hat{\sigma}^z \otimes \mathfrak{e}_j^{(2m)}, \quad j = 1, \ldots, 2m+1. \tag{7}$$

The group $\mathrm{Spin}(n)$ is defined as a subset of $\mathcal{C\ell}(\mathbb{R}, n)$ generated by all possible products of *even* number of elements $\mathfrak{e}(\mathbf{v})$ with different vectors $\mathbf{v}$ of unit length

$$\begin{aligned} \hat{\mathfrak{s}} = \mathfrak{e}(\mathbf{v}_1)\mathfrak{e}(\mathbf{v}_2)\cdots\mathfrak{e}(\mathbf{v}_{2k}), \quad \mathbf{v}_j \in \mathbb{R}^n, \\ |\mathbf{v}_j| = 1, \quad j = 1, \ldots, 2k. \end{aligned} \tag{8}$$

The basic property of $\mathrm{Spin}(n)$ is the expression of orthogonal group as

$$\hat{\mathfrak{s}}\, \mathfrak{e}(\mathbf{v})\, \hat{\mathfrak{s}}^{-1} = \mathfrak{e}(\mathbf{v}'), \quad \mathbf{v}' = \mathsf{R}_{\hat{\mathfrak{s}}}\mathbf{v}, \quad \mathsf{R}_{\hat{\mathfrak{s}}} \in \mathrm{SO}(n), \tag{9}$$

i.e., $\mathsf{R}_{\hat{\mathfrak{s}}}$ is some n-dimensional rotation. It should be noted, that the *two* elements $\pm\hat{\mathfrak{s}} \in \mathrm{Spin}(n)$ in Eq. (9) correspond to *the same* transformation $\mathsf{R}_{\hat{\mathfrak{s}}} \in \mathrm{SO}(n)$. Thus, $\mathrm{Spin}(n)$ group *doubly covers* $\mathrm{SO}(n)$.

The Spin group also can be described as the Lie group. The universal Clifford algebra $\mathcal{C\ell}_n = \mathcal{C\ell}(\mathbb{F}, n)$ is a Lie algebra with respect to the bracket operation

$$[\mathfrak{a}, \mathfrak{b}] = \mathfrak{a}\mathfrak{b} - \mathfrak{b}\mathfrak{a}, \quad \mathfrak{a}, \mathfrak{b} \in \mathcal{C\ell}_n.$$

For the Lie group $\mathrm{Spin}(n)$, the Lie algebra $\mathrm{spin}(n)$ is a subalgebra of $\mathcal{C\ell}_n$ with the basis $\mathfrak{e}_j\mathfrak{e}_k$, $1 \le j < k \le n$. The Lie algebra $\mathrm{so}(n)$ of the orthogonal group is isomorphic with $\mathrm{spin}(n)$.

The representation of $\mathrm{Spin}(n)$ groups using the Clifford algebras discussed above has dimension 2^n, but both $\mathrm{spin}(n)$ and $\mathrm{so}(n)$ have dimension only $n(n-1)/2$. The Lie algebraic approach is also important due to direct relation with Hamiltonians of quantum gates [1, 13].

There is some subtlety, because the exponential map producing an element of the Spin group is $\mathcal{A}_\epsilon = \exp(\epsilon\mathfrak{a})$, but in the physical applications expressions with the generators are often written with an imaginary unit multiplier, *e.g.*, the quantum gates near identity should be written [14]

$$\delta\hat{U} = e^{\imath\epsilon\hat{H}} \simeq \mathbb{1} + \imath\epsilon\hat{H}, \quad \epsilon \to 0. \tag{10}$$

In this case, the imaginary unit should also appear in anticommutators. For example, the commutator algebra with the bracket operation $\imath[\hat{H}_a, \hat{H}_b]$ appears in a proof of two-qubit gates universality [14]. The set of gates represented in such a way is universal if elements $\hat{H}$ from Eq. (10) generate entire Lie algebra of unitary group by the commutators.

Similar Lie-algebraic approach to Clifford algebras can be used for construction of both universal and non-universal sets of two-qubit gates [13]. The basis of the Lie algebra spin$(2m)$ consists of quadratic elements $\mathfrak{e}_j\mathfrak{e}_k$. The construction of the Lie algebra spin$(2m)$ using Eq. (5) represents the Spin$(2m)$ group as some subgroup of the unitary group U(2^m).

Let us consider four consequent generators $\mathfrak{e}_{2k-1}$, $\mathfrak{e}_{2k}$, $\mathfrak{e}_{2k+1}$, $\mathfrak{e}_{2k+2}$. The linear combinations of six different quadratic elements produced from the generators for the particular representation (5) correspond to Hamiltonians of some one- and two-qubit gates. For different k it generates the non-universal set of quantum gates on nearest-neighbor qubits often called *matchgates* [15, 16].

The Jordan–Wigner representation of generators for Clifford algebra (5) is not unique. Alternative methods based on tree-like structures are discussed in next sections.

3 Ternary Trees

Let us consider the following nine generators

$$\begin{aligned}
\tilde{\mathfrak{e}}_1 &= \imath\hat{\sigma}^x \otimes \hat{\sigma}^x \otimes \mathbb{1} \otimes \mathbb{1},\\
\tilde{\mathfrak{e}}_2 &= \imath\hat{\sigma}^x \otimes \hat{\sigma}^y \otimes \mathbb{1} \otimes \mathbb{1},\\
\tilde{\mathfrak{e}}_3 &= \imath\hat{\sigma}^x \otimes \hat{\sigma}^z \otimes \mathbb{1} \otimes \mathbb{1},\\
\tilde{\mathfrak{e}}_4 &= \imath\hat{\sigma}^y \otimes \mathbb{1} \otimes \hat{\sigma}^x \otimes \mathbb{1},\\
\tilde{\mathfrak{e}}_5 &= \imath\hat{\sigma}^y \otimes \mathbb{1} \otimes \hat{\sigma}^y \otimes \mathbb{1},\\
\tilde{\mathfrak{e}}_6 &= \imath\hat{\sigma}^y \otimes \mathbb{1} \otimes \hat{\sigma}^z \otimes \mathbb{1},\\
\tilde{\mathfrak{e}}_7 &= \imath\hat{\sigma}^z \otimes \mathbb{1} \otimes \mathbb{1} \otimes \hat{\sigma}^x,\\
\tilde{\mathfrak{e}}_8 &= \imath\hat{\sigma}^z \otimes \mathbb{1} \otimes \mathbb{1} \otimes \hat{\sigma}^y,\\
\tilde{\mathfrak{e}}_9 &= \imath\hat{\sigma}^z \otimes \mathbb{1} \otimes \mathbb{1} \otimes \hat{\sigma}^z.
\end{aligned} \tag{11}$$

A much more concise notation will be used further

$$\begin{aligned}
&\tilde{\mathfrak{e}}_1 = \imath\hat{\sigma}^x_1\hat{\sigma}^x_2, \quad \tilde{\mathfrak{e}}_2 = \imath\hat{\sigma}^x_1\hat{\sigma}^y_2, \quad \tilde{\mathfrak{e}}_3 = \imath\hat{\sigma}^x_1\hat{\sigma}^z_2,\\
&\tilde{\mathfrak{e}}_4 = \imath\hat{\sigma}^y_1\hat{\sigma}^x_3, \quad \tilde{\mathfrak{e}}_5 = \imath\hat{\sigma}^y_1\hat{\sigma}^y_3, \quad \tilde{\mathfrak{e}}_6 = \imath\hat{\sigma}^y_1\hat{\sigma}^z_3,\\
&\tilde{\mathfrak{e}}_7 = \imath\hat{\sigma}^z_1\hat{\sigma}^x_4, \quad \tilde{\mathfrak{e}}_8 = \imath\hat{\sigma}^z_1\hat{\sigma}^y_4, \quad \tilde{\mathfrak{e}}_9 = \imath\hat{\sigma}^z_1\hat{\sigma}^z_4,
\end{aligned} \tag{11$'$}$$

where $\hat{\sigma}^\mu_j$ denotes Pauli matrix $\mu = x, y, z$ acting on qubit with index j.

The universal Clifford algebra could be defined using eight generators instead of nine and product of all $\tilde{\mathfrak{e}}_k$ is identity up to possible multiplier with some power of the imaginary unit denoted further as

$$\iota \in \{\pm 1, \pm \imath\}, \quad \iota^4 = 1. \tag{12}$$

The nine generators (11) demonstrate natural threefold symmetries derived from Pauli matrices. The generalization for arbitrary power of three using ternary trees is discussed below. For the initial example (11), it corresponds to four qubit nodes $j = 1, \ldots, 4$ represented by lower indices in Eq. (11$'$) where the root is $j = 1$ and the three child nodes $j = 2, 3, 4$ are associated with three generators each. Such construction can be generalized, *e.g.*, similar example with tree for *thirteen qubits* is provided in Fig. 1 with scheme of *twenty seven generators* depicted in Fig. 2.

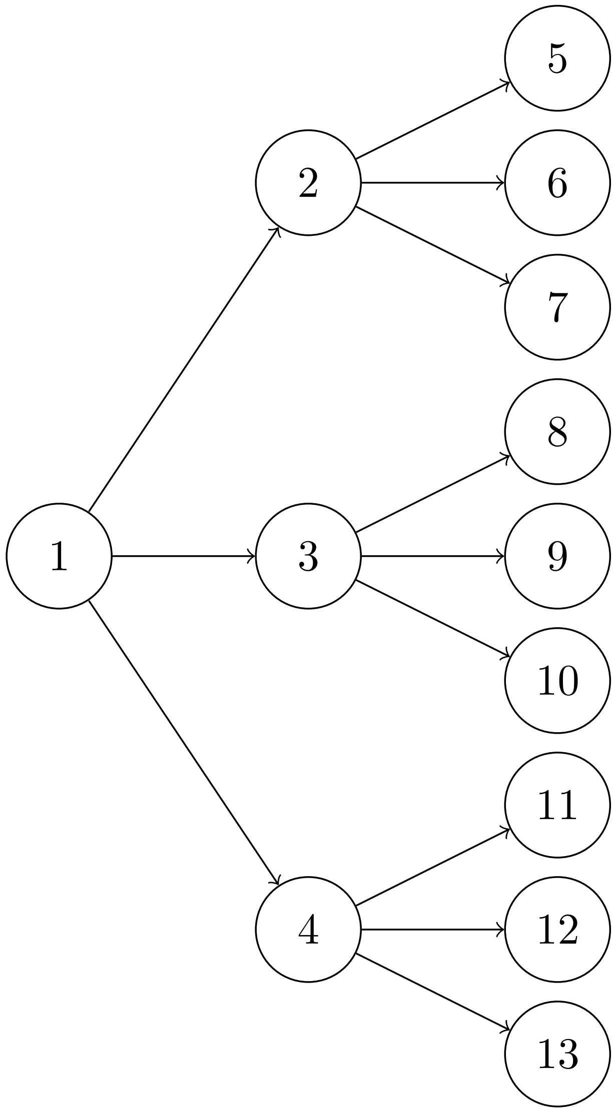

Figure 1: *Ternary* Υ_{L}*-tree with* $\mathsf{L} = 3$.

Let us recollect some useful properties of rooted trees [17, 18]. A node of n-ary tree has up to n children, the nodes without any children are called *terminal* nodes or *leafs*. The *level* ℓ is defined here as the number of nodes in the path from the root. The maximal level of nodes in a tree is denoted further as L and, thus, the *height* of the tree is $\mathsf{L} - 1$.

Ternary or binary trees with maximal number of nodes for given L are denoted here as 'Υ_{L}-trees'. It could be formally described using definitions from Ref. [18] as *directed rooted complete full ternary (or binary) tree with height* $\mathsf{L}-1$. In some constructions below, an auxiliary root with index zero can also be attached to the first node producing trees of height L. Such a method is relevant to Eq. (21) and Eq. (22) below. It is also used for the production of $\Upsilon^{\circ}_{\mathsf{L}}$-tree from Υ_{L}-tree in Section 7.1.

The number of nodes in a *ternary* Υ_{L}-tree is

$$m_{\mathsf{L}} = \sum_{k=0}^{\mathsf{L}-1} 3^k = \frac{3^{\mathsf{L}}-1}{2}. \tag{13}$$

Let us start with three generators $\tilde{\mathbf{e}}^{(3)}_1 = \imath\hat{\sigma}^x$, $\tilde{\mathbf{e}}^{(3)}_2 = \imath\hat{\sigma}^y$, $\tilde{\mathbf{e}}^{(3)}_3 = \imath\hat{\sigma}^z$ for $\mathsf{L}=1$. For any $\mathsf{L}>1$, $3^{\mathsf{L}+1}$ anticommuting generators for ternary $\Upsilon_{\mathsf{L}+1}$-tree can be produced by recursion $\mathsf{L}\to\mathsf{L}+1$ using 3^{L} anticommuting generators defined for Υ_{L}-tree

$$\begin{aligned}
\tilde{\mathbf{e}}^{(3^{\mathsf{L}+1})}_{3j-2} &= \tilde{\mathbf{e}}^{(3^{\mathsf{L}})}_j \otimes \underbrace{\mathbb{1}\otimes\cdots\otimes\mathbb{1}}_{j-1} \otimes \hat{\sigma}^x \otimes \underbrace{\mathbb{1}\otimes\cdots\otimes\mathbb{1}}_{3^{\mathsf{L}}-j},\\
\tilde{\mathbf{e}}^{(3^{\mathsf{L}+1})}_{3j-1} &= \tilde{\mathbf{e}}^{(3^{\mathsf{L}})}_j \otimes \underbrace{\mathbb{1}\otimes\cdots\otimes\mathbb{1}}_{j-1} \otimes \hat{\sigma}^y \otimes \underbrace{\mathbb{1}\otimes\cdots\otimes\mathbb{1}}_{3^{\mathsf{L}}-j},\\
\tilde{\mathbf{e}}^{(3^{\mathsf{L}+1})}_{3j} &= \tilde{\mathbf{e}}^{(3^{\mathsf{L}})}_j \otimes \underbrace{\mathbb{1}\otimes\cdots\otimes\mathbb{1}}_{j-1} \otimes \hat{\sigma}^z \otimes \underbrace{\mathbb{1}\otimes\cdots\otimes\mathbb{1}}_{3^{\mathsf{L}}-j},
\end{aligned} \tag{14}$$

where $j=1,\ldots,3^{\mathsf{L}}$ and the total number of terms in the tensor product is $m_{\mathsf{L}+1} = m_{\mathsf{L}} + 3^{\mathsf{L}}$. All generators in Eq. (14) anticommute — in different triples due to terms $\tilde{\mathbf{e}}^{(3^{\mathsf{L}})}_j$ and in the same triple due to terms $\hat{\sigma}^{\mu}_j$ ($\mu = x,y,z$).

Let us prove recursively that any $3^{\mathsf{L}}-1$ generators between $\tilde{\mathbf{e}}^{(3^{\mathsf{L}})}_j$ generate whole basis for universal Clifford algebra $\mathcal{C}\ell(2m_{\mathsf{L}},\mathbb{C})$. Let us start with a useful property: the product of all 3^{L} generators is $\imath\mathbb{1}$. It is true for $\mathsf{L}=1$, $\tilde{\mathbf{e}}^{(3)}_k$, $k=1,2,3$ and for any $\mathsf{L}+1$ it is derived directly from Eq. (14). Due to this property any chosen generator up to $\imath$ multiplier is represented as a product of all other generators and can be dropped. Thus, any $3^{\mathsf{L}}-1$ generators between 3^{L} can be used as a basis of $\mathcal{C}\ell(2m_{\mathsf{L}},\mathbb{C})$.

The standard basis of $\mathcal{C}\ell(2m_{\mathsf{L}},\mathbb{C})$ is naturally expressed as $4^{m_{\mathsf{L}}}$ tensor products using *Pauli basis*, *i.e.*, three Pauli matrices and 2×2 unit matrix. Let us show, that the basis can also be represented (not necessary in unique way) by products of $\tilde{\mathbf{e}}^{(3^{\mathsf{L}})}_k$. It is again true for $\mathsf{L}=1$ and $\mathcal{C}\ell(2,\mathbb{C})$. Let us consider $\mathsf{L}+1$ for some $\mathsf{L}\geq 1$ with the basis of $\mathcal{C}\ell(2m_{\mathsf{L}},\mathbb{C})$ expressed by products of $\tilde{\mathbf{e}}^{(3^{\mathsf{L}})}_k$. Arbitrary basic element $\mathfrak{b}$ of $\mathcal{C}\ell(2m_{\mathsf{L}+1},\mathbb{C})$ can be represented as tensor products with $m_{\mathsf{L}+1}$ elements of Pauli basis. The product of three generators for any j in Eq. (14) is

$$\imath\,\tilde{\mathbf{e}}^{(3^{\mathsf{L}})}_j \otimes \underbrace{\mathbb{1}\otimes\cdots\otimes\mathbb{1}}_{3^{\mathsf{L}}},$$

so, the first m_{L} terms in $\mathfrak{b}$ can be rewritten by product of such triples due to previous steps of recursion. Three possible products of two generators with given j in Eq. (14) are

$$\imath\,\underbrace{\mathbb{1}\otimes\cdots\otimes\mathbb{1}}_{m_{\mathsf{L}}+j-1} \otimes \hat{\sigma}^{\mu} \otimes \underbrace{\mathbb{1}\otimes\cdots\otimes\mathbb{1}}_{3^{\mathsf{L}}-j}, \quad \mu = x,y,z,$$

and remaining last 3^{L} terms of $\mathfrak{b}$ can also be expressed using products of such pairs. So, any element $\mathfrak{b}$ of standard basis $\mathcal{C}\ell(2m_{\mathsf{L}+1},\mathbb{C})$ with $m_{\mathsf{L}+1} = m_{\mathsf{L}} + 3^{\mathsf{L}}$ terms is some product of $\tilde{\mathbf{e}}^{(3^{\mathsf{L}+1})}_k$.

It was also shown, that any element can be expressed up to $\imath$ as product of other generators. In this case, the construction with one dropped element corresponds to *universal* Clifford algebra. □

Each generator $\tilde{\mathbf{e}}^{(3^{\mathsf{L}})}_k$, $k=1,\ldots,3^{\mathsf{L}}$ has $m_{\mathsf{L}}=(3^{\mathsf{L}}-1)/2$ terms in tensor product with only L (non-unit) Pauli matrices, because recursion (14) appends only one non-unit term for each level. The scheme of such terms may be represented by directed ternary Υ_{L}-tree with first qubit as root, see Fig. 1. Each triple of generators in Eq. (14) formally corresponds to path from the root of the tree to *leaf* nodes.

For example, the tree with three levels represented in Fig. 1 may illustrate structure of nine triples with twenty seven generators: $\tilde{\mathbf{e}}^{(27)}_1 = \imath\hat{\sigma}^x_1\hat{\sigma}^x_2\hat{\sigma}^x_5$, $\tilde{\mathbf{e}}^{(27)}_2 = \imath\hat{\sigma}^x_1\hat{\sigma}^x_2\hat{\sigma}^y_5$, $\tilde{\mathbf{e}}^{(27)}_3 = \imath\hat{\sigma}^x_1\hat{\sigma}^x_2\hat{\sigma}^z_5$, $\tilde{\mathbf{e}}^{(27)}_4 = \imath\hat{\sigma}^x_1\hat{\sigma}^x_2\hat{\sigma}^x_6$, $\ldots$, $\tilde{\mathbf{e}}^{(27)}_{27} = \imath\hat{\sigma}^z_1\hat{\sigma}^z_4\hat{\sigma}^z_{13}$.

The tree representation provides yet another explanation of anticommutativity of all $\tilde{\mathbf{e}}^{(m_{\mathsf{L}})}_j$. Any two 'branches' of tree have some common part corresponding to qubits with the same index and non-unit tensor factors, but only the last pair of Pauli matrices in common subsequences (corresponding to 'fork node' for pair of branches) may differ. Such approach produces an illustrative argument for the generalization with arbitrary ternary trees.

Let us first extend the model to provide formal definition using some methods from the theory of *deterministic finite automata* (DFA) [19,20]. The model of deterministic finite automaton below uses *extension* [17] of ternary Υ_{L}-tree with basic nodes representing qubits and three additional *output nodes* for each leaf. For more general ternary trees discussed further, the number of children for any qubit node is added up to three by new output nodes.

Each link is marked by letters x,y,z representing possible transition between nodes, see Fig. 2. The *word* (sequence of letters x,y,z) corresponding to path from the root to output nodes is *recognized* by deterministic finite automaton. The sequence of nodes generated by such transition represents generator expressed as product of terms with Pauli matrices indexed by the number of node and letter, *e.g.*, $xxx \to \hat{\sigma}^x_1\hat{\sigma}^x_2\hat{\sigma}^x_5$, …, $xyz \to \hat{\sigma}^x_1\hat{\sigma}^y_2\hat{\sigma}^z_6$, …, $zyx \to \hat{\sigma}^z_1\hat{\sigma}^y_4\hat{\sigma}^x_{12}$, …, $zzz \to \hat{\sigma}^z_1\hat{\sigma}^z_4\hat{\sigma}^z_{13}$ for Fig. 2.

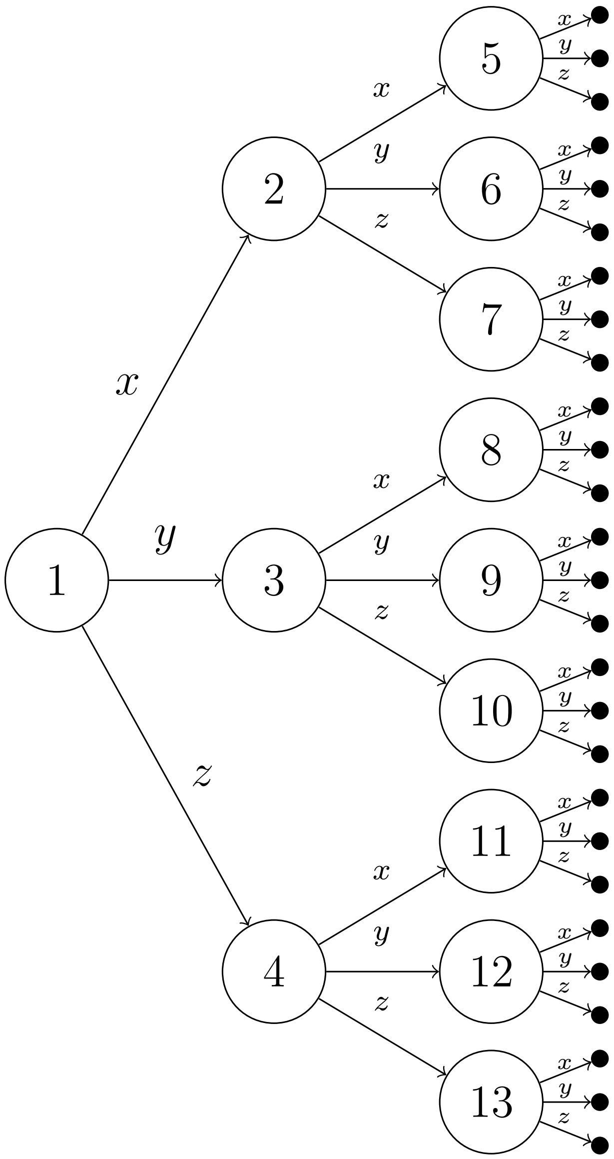

Figure 2: Deterministic finite automaton (DFA) from ternary Υ_{L}*-tree* extended *by leaf nodes.*

More generally, if some sequence $\mu_1\mu_2\ldots\mu_\ell$ of letters $\mu_k \in \{x, y, z\}$ for $k = 1, \ldots, \ell$ is recognized by deterministic finite automaton and generates sequence of nodes (path)

$$j_1 \xrightarrow{\mu_1} j_2 \xrightarrow{\mu_2} \cdots \xrightarrow{\mu_{\ell-1}} j_\ell \xrightarrow{\mu_l} o_{\ell+1} \tag{15}$$

with root $j_1 = 1$ and $o_{\ell+1}$ is the output node, the generator is

$$\tilde{\mathfrak{e}}_{o_{\ell+1}} = \iota\hat{\sigma}^{\mu_1}_{j_1}\hat{\sigma}^{\mu_2}_{j_2}\cdots\hat{\sigma}^{\mu_\ell}_{j_\ell} = \iota\prod_{k=1}^{\ell}\hat{\sigma}^{\mu_k}_{j_k}. \tag{16}$$

The model with deterministic finite automaton and Eq. (16) can be applied for a general ternary tree for a level ℓ that is not necessary equal to the maximal L and the number of outbound links for each node may be from zero to three. Let us start with a ternary Υ_{L}-tree discussed above with maximal number of qubit nodes $m_{\rm q} = (3^{\mathsf{L}} - 1)/2$ and $n_{\rm g} = 3^{\mathsf{L}}$ anticommuting generators

$$n_{\rm g} = 2m_{\rm q} + 1. \tag{17}$$

Eq. (17) is also valid for any subtree.

Other ternary trees can be produced by recursive process of 'pruning' discussed below. Let us delete all nodes and generators of subtree $\boldsymbol{\varsigma}$ originated from node $j_{\boldsymbol{\varsigma}}$ attached to parent node j_p by link with label $\mu_p \in \{x, y, z\}$. Let us also add the new element including only initial common sequence of nodes in products (16) coinciding for all deleted nodes of the subtree $\boldsymbol{\varsigma}$

$$\tilde{\mathfrak{e}}_{\boldsymbol{\varsigma}} = \iota\hat{\sigma}^{\mu_1}_1\cdots\hat{\sigma}^{\mu_p}_{j_p}. \tag{18}$$

The tree and all its subtrees after any deletion also satisfy Eq. (17), because

$$n'_{\rm g} = n_{\rm g} - n^{\boldsymbol{\varsigma}}_{\rm g} + 1 = (2m_{\rm q} + 1) - (2m^{\boldsymbol{\varsigma}}_{\rm q} + 1) + 1 = 2m'_{\rm q} + 1,$$

where $n'_{\rm g}$, $m'_{\rm q}$ and $n^{\boldsymbol{\varsigma}}_{\rm g}$, $m^{\boldsymbol{\varsigma}}_{\rm q}$ denote parameters (number of generators, number of qubit nodes) for produced tree and deleted subtree respectively.

The new element (18) anticommutes with all elements except deleted ones. Let us also prove that the product of $n'_{\rm g}$ generators for the new tree is $\iota\mathbb{1}$, where ι is possible unessential multiplier (12). For the initial ternary Υ_{L}-tree, Eq. (17) holds true and the product of all generators was already calculated earlier. Any subtree of the Υ_{L}-tree is also ternary $\Upsilon_{\mathsf{L}'}$-tree for some $\mathsf{L}' < \mathsf{L}$ and the product of all generators for such subtree is

$$\prod_{k\in\boldsymbol{\varsigma}}\tilde{\mathfrak{e}}_k = (\tilde{\mathfrak{e}}_{\boldsymbol{\varsigma}})^{n^{\boldsymbol{\varsigma}}_{\rm g}}(\pm\mathbb{1}) = \mp\tilde{\mathfrak{e}}_{\boldsymbol{\varsigma}},$$

because $n^{\boldsymbol{\varsigma}}_{\rm g}$ is odd and $(\tilde{\mathfrak{e}}_{\boldsymbol{\varsigma}})^2 = -1$. So, after each deletion the products of all generators of *deleted trees* up to sign are equal with corresponding $\tilde{\mathfrak{e}}_{\boldsymbol{\varsigma}}$ and the total product of *all elements* is always $\iota\mathbb{1}$.

Let us prove, that for any tree with $m'_{\rm q}$ qubit nodes obtained by such pruning, the products of any subset with $n'_{\rm g} - 1 = 2m'_{\rm q}$ generators may be used as a basis of universal Clifford algebra $\boldsymbol{C\ell}(2m'_{\rm q}, \mathbb{C})$. Let us again for simplicity start with all $n'_{\rm g} = 2m'_{\rm q} + 1$ generators, because any generator may be expressed as a product of other generators.

Let us note, that each deletion in the process of pruning may be treated also as a two-stage process: (1) to drop multipliers with Pauli matrices for excluded qubit nodes from all products and (2) to remove duplicates from the list of generators. The approach is also correct for description of whole pruning as a series of consequent deletions.

Let us consider the final tree as a subtree of ternary Υ_{L}-tree. Any element of standard basis of the Clifford algebra for qubits from this subtree can be represented by product of generators of the initial tree. If when dropping Pauli matrices for extra qubits from generators in such products the result may only change sign, now it includes only terms that are equal with generators of subtree. Thus, the resulting terms provide a basis of the Clifford algebra for the final tree. □

Let us describe formal procedure for construction of generators from arbitrary ternary tree produced by the pruning described above:

- Ternary tree should be extended by adding of *terminal* (output) nodes, *i.e.*, all initial nodes with number of children $n_c < 3$ should be connected with $3 - n_c$ new leafs associated with generators.
- Now all non-terminal (initial) nodes have three output links marked by triple of labels x, y, z. Such a tree also may be considered as a deterministic finite automaton.
- Any path from the root to terminal node is described by an analogue of Eq. (15) where l is the level of the node and the generator for each terminal node can be expressed as Eq. (16).
- Formally, a possible sequence of letters $\mu_k \in \{x, y, z\}$ in Eq. (15) corresponds to *a word recognized by the deterministic finite automaton* and any generator is represented in such a way by product of Pauli matrices (16).

Let us summarize the construction of generators using an *extended ternary tree*. Rooted directed ternary tree is defined by set of qubit nodes $j = 1, \ldots, m$ and directed links between pairs of nodes. Any node except the root has one parent and up to three children. The links are marked by labels x, y, z.

Let us first define an auxiliary operator (*stub*) $\hat{\mathfrak{r}}_j$ for any qubit node j. For the root node $j = 1$, $\hat{\mathfrak{r}}_1 = \imath\mathbb{1}$ and for any child node k linked with a parent node j by link with a label $\mu \in \{x, y, z\}$

$$j \xrightarrow{\mu} k: \quad \hat{\mathfrak{r}}_k = \hat{\mathfrak{r}}_j \hat{\sigma}^{\mu}_j. \tag{19}$$

Now for any node j with less than three children n_c, it is necessary to attach $n_o = 3 - n_c$ *output* generator nodes with appropriate unique indices $\tilde{\jmath}$ by new links for missing labels $\mu \in \{x, y, z\}$.

The maximal total number of outbound links for m nodes is $3m$, but $m - 1$ children are qubit nodes (because all of them except the root have one parent). Thus, the number of generator nodes satisfies Eq. (17)

$$n_g = 3m - (m - 1) = 2m + 1.$$

The generator associated with each such node is defined as

$$\tilde{\mathbf{e}}_{\tilde{\jmath}} = \tilde{\mathbf{e}}_{j;\mu} = \hat{\mathfrak{r}}_j \hat{\sigma}^{\mu}_j, \quad \tilde{\jmath} = 1, \ldots, 2m + 1, \quad j = 1, \ldots, m. \tag{20}$$

An alternative notation $\tilde{\mathbf{e}}_{j;\mu}$ is introduced for convenience in Eq. (20). Any generator may be expressed in this way $\tilde{\mathbf{e}}_{\tilde{\jmath}} = \tilde{\mathbf{e}}_{j;\mu}$ after choosing of some map to set the consequent indices $\tilde{\jmath} = \tilde{\jmath}(j, \mu)$, but the number of elements $\tilde{\mathbf{e}}_{j;\mu}$ is bigger, $3m > 2m + 1$. Redundant $\tilde{\mathbf{e}}_{j;\mu}$ correspond to products of generators denoted earlier as $\tilde{\mathbf{e}}_{\varsigma}$ (18). □

Eq. (20) together with the definition of stub operator (19) formalizes Eq. (16) used earlier without necessity to introduce an enveloping Υ_{L}-tree.

For the ternary Υ_{L}-tree, deterministic finite automaton recognizes any sequences with L letters and the resulting 3^{L} generators are attached to leafs of the qubit tree shown in Fig. 2. The number of nodes for such a tree is $(3^{\mathsf{L}} - 1)/2$ according to Eq. (13).

For more general ternary tree with m nodes produced with the method discussed above, the number of generator leafs (DFA output nodes) on the extended tree is always $2m + 1$. The product of all generators is proportional to identity. It was already discussed that any subset with $2m$ generators may be used for construction of universal Clifford algebra $\mathcal{C}\ell(2m, \mathbb{C})$.

Let us consider yet another formal construction of $\mathcal{C}\ell(2m + 1, \mathbb{C})$ without necessity to get rid of one generator. Let us introduce an auxiliary node with index zero to extend the set of generators to $m + 1$ qubits using a straightforward method, *cf* Eq. (7)

$$\acute{\mathbf{e}}_j = \hat{\sigma}^z \otimes \tilde{\mathbf{e}}_j, \quad j = 1, \ldots, 2m + 1. \tag{21}$$

The products of $2m + 1$ elements (21) is $\hat{\sigma}^z_0$ and, thus, $\mathcal{C}\ell(2m + 1, \mathbb{C})$ can be generated by Eq. (21) using standard representation with block diagonal matrices, see Eq. (6).

The *even subalgebra* $\mathcal{C}\ell_0$ is generated by products of even number of generators $\acute{\mathbf{e}}_j$ (21). The cancellation of $\hat{\sigma}^z_0$ in products illustrates natural isomorphism

$$\mathcal{C}\ell_0(2m + 1, \mathbb{C}) \simeq \mathcal{C}\ell(2m, \mathbb{C})$$

and it also produces representation of $\mathrm{Spin}(2m + 1)$ group by all $2m + 1$ elements $\tilde{\mathbf{e}}_j \in \mathcal{C}\ell(2m, \mathbb{C})$.

For $m > 1$, the $\mathrm{Spin}(2m+2)$ can also be represented in a similar way. Let us consider construction of Spin groups as Lie algebras [11] recollected in Section 2. In this case, the element may be expressed as an exponent of linear combinations of quadratic terms $\mathfrak{e}_j\mathfrak{e}_k$.

Let us again introduce an extra zero node, but for an alternative representation of $2m+2$ generators instead of Eq. (21) should be used the following

$$\begin{aligned} \grave{\mathfrak{e}}_j &= \hat{\sigma}^x \otimes \tilde{\mathfrak{e}}_j, \qquad j = 1,\dots,2m+1, \\ \grave{\mathfrak{e}}_0 &= \hat{\sigma}^y \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1}. \end{aligned} \tag{22}$$

The products of two such elements are either $\mathbb{1} \otimes (\tilde{\mathfrak{e}}_j\tilde{\mathfrak{e}}_k)$ or $\hat{\sigma}^z \otimes \tilde{\mathfrak{e}}_l$, where $j,k,l = 1,\dots,2m+1$. The quadratic terms can be expressed as block-diagonal matrices (6). For $m > 1$ all $\tilde{\mathfrak{e}}_j\tilde{\mathfrak{e}}_k$ with $j < k$ and $\tilde{\mathfrak{e}}_l$ are different and exponents of matrices with linear combination of such elements $\exp(\mathbf{A}) \in \mathcal{C}\ell(2m,\mathbb{C})$ can be used for construction of irreducible representation of $\mathrm{Spin}(2m+2)$. It is not true for $m = 1$ due to $\tilde{\mathfrak{e}}_1\tilde{\mathfrak{e}}_2 = \tilde{\mathfrak{e}}_3$, *e.g.*, for quaternions or Pauli matrices $\hat{\sigma}_x\hat{\sigma}_y = \imath\hat{\sigma}_z$.

A standard representation of Clifford algebra may be considered as an extreme case of pruning into a chain of z-linked nodes. At least two generators (x, y) are attached to each node with an additional one (z) on the end. Such a degenerate tree corresponds to $2m$ Jordan–Wigner generators (5)

$$\begin{aligned} \mathfrak{e}_{2k-1} &= \imath\hat{\sigma}^z_1 \cdots \hat{\sigma}^z_{k-1}\,\hat{\sigma}^x_k \\ \mathfrak{e}_{2k} &= \imath\hat{\sigma}^z_1 \cdots \hat{\sigma}^z_{k-1}\,\hat{\sigma}^y_k \end{aligned}$$

for $k = 1,\dots,m$ together with Eq. (5′)

$$\mathfrak{e}_{2m+1} = \imath\hat{\sigma}^z_1 \cdots \hat{\sigma}^z_{2m}.$$

4 Binary Trees

Binary Υ_{L}-trees can be introduced formally by deletion of all nodes attached to z-links of the ternary Υ_{L}-trees, see Fig. 3. The term *binary x-y tree* may be also used sometimes to distinguish that from an alternative construction with deleted y-links, but such 'x-z trees' are introduced only in Section 7.1.

The deterministic finite automaton for such binary tree produces three generators for terminal qubit nodes with maximal level $l = \mathsf{L}$, but only one generator for other qubit nodes with $l < \mathsf{L}$, see Fig. 4.

The binary Υ_{L}-tree has $2^{\mathsf{L}} - 1$ qubit nodes. With 'enumeration along levels' the nodes $j = 1,\dots,2^{\mathsf{L}-1} - 1$ have two children $2j$ and $2j+1$, except leafs $j = 2^{\mathsf{L}-1},\dots,2^{\mathsf{L}} - 1$, see Fig. 5.

The *stub operator* $\hat{\mathfrak{r}}_j$ (19) used for construction of generators (20) can be constructed for binary case in the similar way as $\hat{\mathfrak{r}}_1 = \imath\mathbb{1}$ and

$$\hat{\mathfrak{r}}_{2j} = \hat{\mathfrak{r}}_j\hat{\sigma}^x_j, \quad \hat{\mathfrak{r}}_{2j+1} = \hat{\mathfrak{r}}_j\hat{\sigma}^y_j. \tag{23}$$

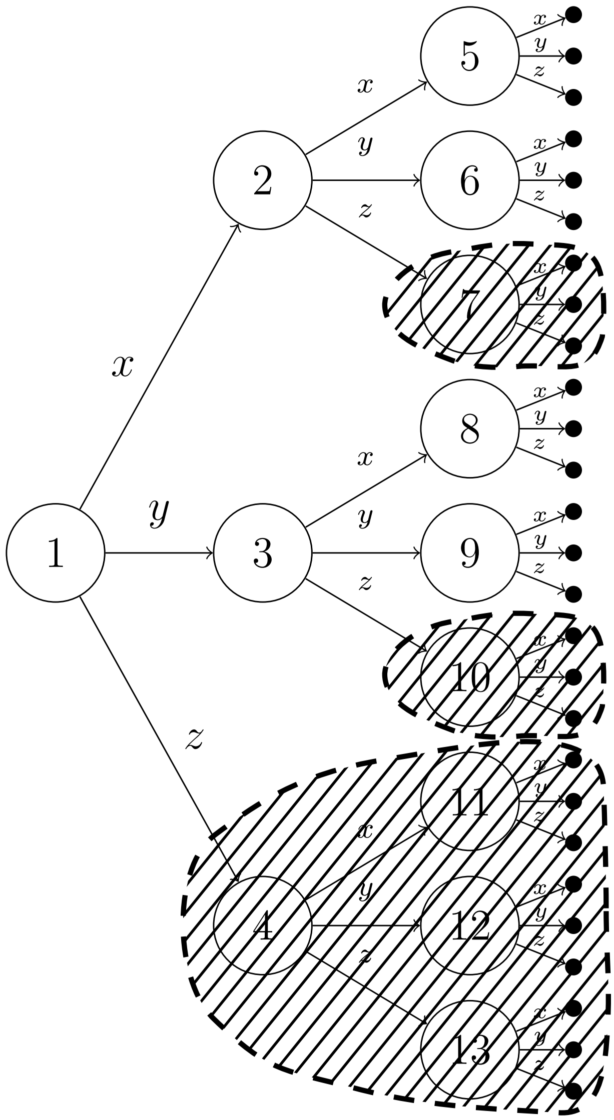

Figure 3: *Binary* (x-y) *tree obtained from the ternary tree shown in Fig. 2.*

For the binary tree with $m_{\mathrm{q}} = 2^{\mathsf{L}} - 1$ qubits discussed earlier, the structure of generators is described by extension into a *ternary* tree, see Fig. 4. Qubits with indices $j = 1,\dots,2^{\mathsf{L}-1} - 1$ have only one generator node, but three generators are linked to the remaining $2^{\mathsf{L}-1}$ terminal qubit nodes $k = 2^{\mathsf{L}-1},\dots,2^{\mathsf{L}} - 1$ with maximal level L. Thus, the total number of generators satisfies Eq. (17)

$$n_g = 2^{\mathsf{L}-1} - 1 + 3 \cdot 2^{\mathsf{L}-1} = 2^{\mathsf{L}+1} - 1 = 2m_{\mathrm{q}} + 1.$$

Here the 'redundant' notation for generators used in Eq. (20) may be more illustrative

$$\tilde{\mathfrak{e}}_{j;z} = \hat{\mathfrak{r}}_j\hat{\sigma}^z_j, \qquad j = 1,\dots,2^{\mathsf{L}-1} - 1, \tag{24a}$$

$$\tilde{\mathfrak{e}}_{j;\mu} = \hat{\mathfrak{r}}_j\hat{\sigma}^\mu_j, \qquad j = 2^{\mathsf{L}-1},\dots,2^{\mathsf{L}} - 1, \quad \mu = x,y,z. \tag{24b}$$

For the binary tree with $\mathsf{L} = 2$ and three qubits, seven

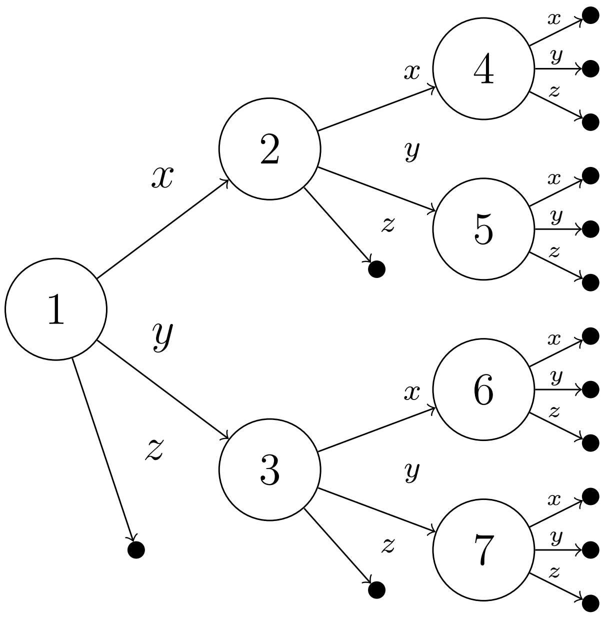

Figure 4: *Deterministic finite automaton (DFA) for a binary tree with additional leaf nodes.*

generators can be written as

$$\tilde{\mathbf{e}}_{1;z} = \imath\hat{\sigma}^z_1, \quad \tilde{\mathbf{e}}_{2;\mu} = \imath\hat{\sigma}^x_1\hat{\sigma}^\mu_2, \quad \tilde{\mathbf{e}}_{3;\mu} = \imath\hat{\sigma}^y_1\hat{\sigma}^\mu_3, \\ \mu = x, y, z. \tag{25}$$

The sequence of terms with index z from Eq. (24) can also be extended to all qubits. Let us use notation $\check{\mathbf{e}}_j$ or $\check{\mathbf{e}}^{(n_\mathrm{g})}_j$, $j = 1, \ldots, n_\mathrm{g} = 2^{\mathsf{L}+1} - 1$ for generators with a consequent indexing with ranges

$$\check{\mathbf{e}}^{(n_\mathrm{g})}_j = \tilde{\mathbf{e}}_{j;z}, \qquad j = 1, \ldots, 2^{\mathsf{L}} - 1, \tag{26a}$$

$$\left.\begin{aligned} \check{\mathbf{e}}^{(n_\mathrm{g})}_{2j} &= \tilde{\mathbf{e}}_{j;x} \\ \check{\mathbf{e}}^{(n_\mathrm{g})}_{2j+1} &= \tilde{\mathbf{e}}_{j;y} \end{aligned}\right\} \qquad j = 2^{\mathsf{L}-1}, \ldots, 2^{\mathsf{L}} - 1. \tag{26b}$$

Thus, for the binary tree with three qubits, Eq. (25) can be rewritten

$$\begin{aligned} \check{\mathbf{e}}^{(7)}_1 = \imath\hat{\sigma}^z_1, \quad \check{\mathbf{e}}^{(7)}_2 &= \imath\hat{\sigma}^x_1\hat{\sigma}^z_2, \quad \check{\mathbf{e}}^{(7)}_3 = \imath\hat{\sigma}^y_1\hat{\sigma}^z_3, \\ \check{\mathbf{e}}^{(7)}_4 &= \imath\hat{\sigma}^x_1\hat{\sigma}^x_2, \quad \check{\mathbf{e}}^{(7)}_5 = \imath\hat{\sigma}^x_1\hat{\sigma}^y_2, \\ \check{\mathbf{e}}^{(7)}_6 &= \imath\hat{\sigma}^y_1\hat{\sigma}^x_3, \quad \check{\mathbf{e}}^{(7)}_7 = \imath\hat{\sigma}^y_1\hat{\sigma}^y_3. \end{aligned} \tag{27}$$

The indexing (26) is convenient due to properties of triples with generators $\check{\mathbf{e}}_j$, $\check{\mathbf{e}}_{2j}$, $\check{\mathbf{e}}_{2j+1}$. Let us denote

$$\hat{\mathfrak{h}}^x_j = \imath\check{\mathbf{e}}_{2j+1}\check{\mathbf{e}}_j, \quad \hat{\mathfrak{h}}^y_j = \imath\check{\mathbf{e}}_j\check{\mathbf{e}}_{2j}, \quad \hat{\mathfrak{h}}^z_j = \imath\check{\mathbf{e}}_{2j}\check{\mathbf{e}}_{2j+1}, \\ j = 1, \ldots, 2^{\mathsf{L}} - 1. \tag{28}$$

The terms (28) are trivial for index j corresponding to terminal qubit nodes with three generators

$$\hat{\mathfrak{h}}^\mu_j = \hat{\sigma}^\mu_j, \quad j = 2^{\mathsf{L}-1}, \ldots, 2^{\mathsf{L}} - 1, \quad \mu = x, y, z. \tag{29}$$

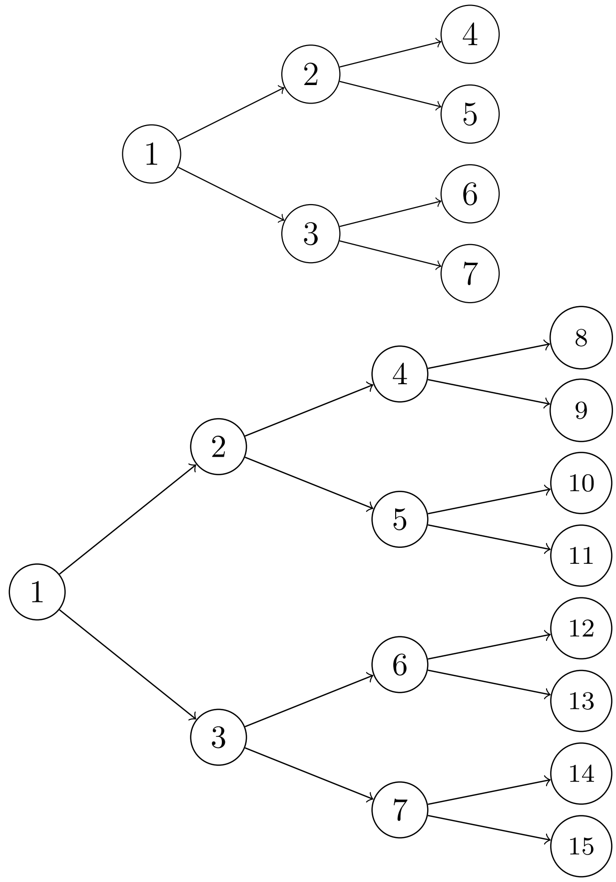

Figure 5: *Binary Υ_{L}-trees for $\mathsf{L} = 3$ and $\mathsf{L} = 4$.*

For nodes with single generator, the first pair of expressions (28) can be associated with links of binary tree

$$\hat{\mathfrak{h}}^y_j = \hat{\sigma}^y_j\hat{\sigma}^z_{2j}, \quad \hat{\mathfrak{h}}^x_j = \hat{\sigma}^x_j\hat{\sigma}^z_{2j+1}, \quad j = 1, \ldots, 2^{\mathsf{L}-1} - 1. \tag{30}$$

It should be noted, that $\hat{\mathfrak{h}}^x_j$ and $\hat{\mathfrak{h}}^y_j$ in Eq. (30) correspond to links marked by exchanged labels (y and x respectively, see Fig. 4). Remaining z-elements in Eq. (28) can be assigned to 'forks' with both links

$$\hat{\mathfrak{h}}^z_j = \hat{\sigma}^z_j\hat{\sigma}^z_{2j}\hat{\sigma}^z_{2j+1}, \quad j = 1, \ldots, 2^{\mathsf{L}-1} - 1. \tag{31}$$

Due to the Lie-algebraic approach, the linear combinations of quadratic expressions such as Eq. (28) correspond to the Hamiltonians $\check{H}$ and the quantum gates can be represented as exponents

$$\check{U} = e^{-\imath\check{H}\tau} = \exp\Bigl(\tau\sum_{j<k} h_{jk}\check{\mathbf{e}}_j\check{\mathbf{e}}_k\Bigr). \tag{32}$$

The Hamiltonians such as Eq. (29) and Eq. (30) generate one- and two-qubit gates and produce non-universal set of quantum gates for representation of Spin group corresponding to Eq. (32). The arbitrary one-qubit gates may be generated by such a way for all terminal qubit nodes due to Eq. (29), but two-qubit gates defined on all links of binary qubit tree are restricted by single-parameter families with Hamiltonians from Eq. (30).

5 Annihilation and creation operators

Let us split $2m$ generators $\mathfrak{e}_j$ of some Clifford algebra $\mathcal{C}\ell(2m,\mathbb{C})$ into two parts with m elements $\mathfrak{e}'_j$, $\mathfrak{e}''_j$ to introduce *annihilation and creation* ('ladder') operators

$$\hat{\mathfrak{a}}_j = \frac{\mathfrak{e}'_j + \imath\mathfrak{e}''_j}{2\imath}, \quad \hat{\mathfrak{a}}^\dagger_j = \frac{\mathfrak{e}'_j - \imath\mathfrak{e}''_j}{2\imath}, \qquad j = 1,\ldots,m. \quad (33)$$

Due to Eq. (3) the elements satisfy *canonical anticommutation relations*

$$\{\hat{\mathfrak{a}}_j, \hat{\mathfrak{a}}_k\} = \{\hat{\mathfrak{a}}^\dagger_j, \hat{\mathfrak{a}}^\dagger_k\} = 0, \quad \{\hat{\mathfrak{a}}_j, \hat{\mathfrak{a}}^\dagger_k\} = \delta_{jk}\mathbb{1}, \quad (34)$$

where $j,k = 1,\ldots,m$.

For the standard representation of Clifford algebra mentioned earlier (5) only the first $2m$ generators may be used $\mathfrak{e}'_j = \mathfrak{e}_{2j-1}$, $\mathfrak{e}''_j = \mathfrak{e}_{2j}$ and thus

$$\hat{\mathfrak{a}}_j = \hat\sigma^z_1 \cdots \hat\sigma^z_{j-1}\,\hat{a}_j, \quad \hat{\mathfrak{a}}^\dagger_j = \hat\sigma^z_1 \cdots \hat\sigma^z_{j-1}\,\hat{a}^\dagger_j, \quad (35)$$

where $j = 1,\ldots,m$ and $\hat{a}$, $\hat{a}^\dagger$ are 2×2 matrices

$$\begin{aligned} \hat{a} &= \frac{\hat\sigma^x + \imath\hat\sigma^y}{2} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \\ \hat{a}^\dagger &= \frac{\hat\sigma^x - \imath\hat\sigma^y}{2} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \end{aligned} \quad (36)$$

with index j is for position in tensor product, *i.e.*,

$$\hat{a}_j \equiv \underbrace{\mathbb{1}\otimes\cdots\otimes\mathbb{1}}_{j-1} \otimes \hat{a} \otimes \underbrace{\mathbb{1}\otimes\cdots\otimes\mathbb{1}}_{m-j}.$$

The usual Jordan–Wigner transformation [2] corresponds to the standard representation (5).

Let us also introduce an analogous notation $\hat{n}_k$, $\hat{n}^0_k$, where

$$\begin{aligned} \hat{n} = \hat{a}^\dagger\hat{a} &= \frac{\mathbb{1} - \hat\sigma^z}{2} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \\ \hat{n}^0 = \hat{a}\hat{a}^\dagger &= \frac{\mathbb{1} + \hat\sigma^z}{2} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \end{aligned} \quad (37)$$

Sometimes in physical applications the ladder operators may be considered as primary objects and expressions for generators follow directly from Eq. (33)

$$\mathfrak{e}'_j = \imath(\hat{\mathfrak{a}}_j + \hat{\mathfrak{a}}^\dagger_j), \quad \mathfrak{e}''_j = \hat{\mathfrak{a}}_j - \hat{\mathfrak{a}}^\dagger_j. \quad (38)$$

The generator $\mathfrak{e}_j$ itself due to such representation is also often treated as a creation operator for a particle coinciding with own antiparticle, *e.g.*, *Majorana mode* [10,21].

The ladder operators also can be used to express specific subgroup of Spin group corresponding to some quantum gates generated by *restricted* set of quadratic Hamiltonians [1,16]. Let us introduce the notation

$$\hat\Sigma_{j,k} = \frac{\hat{\mathfrak{a}}^\dagger_j\hat{\mathfrak{a}}_k + \hat{\mathfrak{a}}^\dagger_k\hat{\mathfrak{a}}_j}{2}, \quad \hat\Lambda_{j,k} = \frac{\hat{\mathfrak{a}}^\dagger_j\hat{\mathfrak{a}}_k - \hat{\mathfrak{a}}^\dagger_k\hat{\mathfrak{a}}_j}{2\imath}. \quad (39)$$

For the 'vacuum' state

$$|\varnothing\rangle \equiv |\underbrace{00\ldots0}_{m}\rangle, \quad (40)$$

$\hat{\mathfrak{a}}_k|\varnothing\rangle = 0$ and thus, $\hat\Sigma_{j,k}|\varnothing\rangle = \hat\Lambda_{j,k}|\varnothing\rangle = 0$. Any Hamiltonian $\hat{\mathcal{H}}$ expressed as a linear combination of Eq. (39) also has the same property $\hat{\mathcal{H}}|\varnothing\rangle = 0$ and the quantum gate generated by such Hamiltonian for some parameter τ

$$\hat{\mathcal{U}} = \exp(-\imath\hat{\mathcal{H}}\tau) \quad (41)$$

does not change the vacuum state $\hat{\mathcal{U}}|\varnothing\rangle = |\varnothing\rangle$.

Let us define consequent indices $1 \le j < k \le m$ in Eq. (39) with special notation for *'occupation number'* operators $\hat{\mathfrak{n}}_k$ and *number of 'particles'* (units in the computational basis) operator $\hat{\mathcal{N}}$

$$\hat{\mathfrak{n}}_k = \hat\Sigma_{k,k} = \hat{\mathfrak{a}}^\dagger_k\hat{\mathfrak{a}}_k, \quad \hat{\mathcal{N}} = \sum_{j=k}^{m} \hat{\mathfrak{n}}_k. \quad (42)$$

An important property of the operator (42) can be derived directly from the definition and Eq. (34)

$$\begin{aligned} \hat{\mathcal{N}}\hat{\mathfrak{a}}_j = \hat{\mathfrak{a}}_j\hat{\mathcal{N}} - \hat{\mathfrak{a}}_j &= \hat{\mathfrak{a}}_j(\hat{\mathcal{N}} - \mathbb{1}), \\ \hat{\mathcal{N}}\hat{\mathfrak{a}}^\dagger_j &= \hat{\mathfrak{a}}^\dagger_j(\hat{\mathcal{N}} + \mathbb{1}). \end{aligned} \quad (43)$$

Here again $\hat{\mathcal{N}}|\varnothing\rangle = 0$ and for states such as

$$\begin{aligned} |\Xi^{(N)}_{j_1\ldots j_N}\rangle &= \underbrace{\hat{\mathfrak{a}}^\dagger_{j_N}\cdots\hat{\mathfrak{a}}^\dagger_{j_1}}_{N}|\varnothing\rangle, \\ 1 \le j_1 &< \cdots < j_N \le m \end{aligned} \quad (44)$$

from consequent application of Eq. (43) for all $\hat{\mathfrak{a}}^\dagger_j$ it follows that

$$\hat{\mathcal{N}}|\Xi^{(N)}_{j_1\ldots j_N}\rangle = N|\Xi^{(N)}_{j_1\ldots j_N}\rangle. \quad (45)$$

It may be also derived from Eq. (43) or checked directly that the quadratic operators (39) commute with N

$$\hat\Sigma_{j,k}\hat{\mathcal{N}} = \hat{\mathcal{N}}\hat\Sigma_{j,k}, \quad \hat\Lambda_{j,k}\hat{\mathcal{N}} = \hat{\mathcal{N}}\hat\Lambda_{j,k}. \quad (46)$$

The Hamiltonian $\hat{\mathcal{H}}$ with linear combination of terms (39) also commutes with $\hat{\mathcal{N}}$ and the quantum gate $\hat{\mathcal{U}}$ generated by $\hat{\mathcal{H}}$ (41) respects subspaces composed from states (44). Such *restricted case* was introduced initially in Ref. [16] and later discussed as a basic example in Ref. [1].

With the standard representation (35), the expression for $\hat{\mathcal{N}}$ (42) may be rewritten as

$$\hat{\mathcal{N}} = \hat{\mathcal{N}}^z \doteq \sum_{k=1}^{m} \hat{\mathfrak{n}}_k = \sum_{k=1}^{m} \frac{\mathbb{1} - \hat{\sigma}^z_k}{2} = \frac{m}{2}\mathbb{1} - \frac{1}{2}\sum_{k=1}^{m} \hat{\sigma}^z_k \quad (47)$$

and the eigenvalues N (45) of the operator correspond to the number of units in the computational basis, *e.g.*, for $N^z = 1$ there are m states

$$|\Xi^{(m)}_k\rangle = \hat{\mathfrak{a}}^\dagger_k|\varnothing\rangle = |\underline{k}\rangle, \quad (48)$$

where, for the standard (Jordan–Wigner) representation we have

$$|\underline{k}\rangle = |\underbrace{0\ldots0}_{k-1}1\underbrace{0\ldots0}_{m-k}\rangle, \quad k = 1,\ldots,m \quad (49)$$

with only unit in position k of the computational basis state, but the analogous constructions even for a binary tree discussed below are more complicated.

Let us now introduce similar constructions for a *binary tree*. The indexation (26) is used further with first element $\check{\mathfrak{e}}_1$ dropped and Eq. (33) is applied to partition $\mathfrak{e}'_j = \check{\mathfrak{e}}_{2j}$, $\mathfrak{e}''_j = \check{\mathfrak{e}}_{2j+1}$, $j = 1,\ldots,m$. Let us also introduce slightly different notation for binary tree ladder operators

$$\check{\mathfrak{a}}_j = \frac{\check{\mathfrak{e}}_{2j} + \imath\check{\mathfrak{e}}_{2j+1}}{2\imath}, \quad \check{\mathfrak{a}}^\dagger_j = \frac{\check{\mathfrak{e}}_{2j} - \imath\check{\mathfrak{e}}_{2j+1}}{2\imath} \quad (50)$$

with $j = 1,\ldots,m$.

Only for the terminal nodes $j = 2^{\mathsf{L}-1},\ldots,2^{\mathsf{L}}-1$ of the binary tree with given L, the operators (50) have more usual form with tensor product of only 2×2 matrices similarly to Eq. (35). Let us consider the simple example with $\mathsf{L} = 2$ (27) where the first node $j = 1$ is not terminal

$$\check{\mathfrak{a}}_1 = \frac{\hat{\sigma}^x_1\hat{\sigma}^z_2 + \imath\hat{\sigma}^y_1\hat{\sigma}^z_3}{2}, \quad \check{\mathfrak{a}}^\dagger_1 = \frac{\hat{\sigma}^x_1\hat{\sigma}^z_2 - \imath\hat{\sigma}^y_1\hat{\sigma}^z_3}{2}. \quad (51)$$

Other operators for $\mathsf{L} = 2$ corresponds to terminal nodes with simpler expressions

$$\begin{aligned}\check{\mathfrak{a}}_2 &= \frac{\hat{\sigma}^x_1\hat{\sigma}^x_2 + \imath\hat{\sigma}^x_1\hat{\sigma}^y_2}{2} = \hat{\sigma}^x_1\hat{a}_2,\\ \check{\mathfrak{a}}_3 &= \frac{\hat{\sigma}^y_1\hat{\sigma}^x_3 + \imath\hat{\sigma}^y_1\hat{\sigma}^y_3}{2} = \hat{\sigma}^y_1\hat{a}_3.\end{aligned} \quad (52)$$

The expressions for operators $\check{\mathfrak{a}}^\dagger_j$ are complex conjugations of matrices and often omitted further. Let us rewrite Eq. (51) using projectors (37)

$$\begin{aligned}\check{\mathfrak{a}}_1 &= \hat{\sigma}^x_1(\hat{n}^0_2 - \hat{n}_2)(\hat{n}^0_3 + \hat{n}_3) + \imath\hat{\sigma}^y_1(\hat{n}^0_2 + \hat{n}_2)(\hat{n}^0_3 - \hat{n}_3)\\ &= \hat{a}_1\hat{n}^0_2\hat{n}^0_3 + \hat{a}^\dagger_1\hat{n}^0_2\hat{n}_3 - \hat{a}^\dagger_1\hat{n}_2\hat{n}^0_3 - \hat{a}_1\hat{n}_2\hat{n}_3.\end{aligned} \quad (53)$$

The expression corresponds to *'conditional' annihilation and creation operators* on the first qubit controlled by a pair of other qubits. The more general case discussed below for $\mathsf{L} \geq 2$ and $j \geq 1$ is quite similar with appropriate indices substituted instead of $1, 2, 3$ in Eq. (53).

Let us rewrite Eq. (50) with two ranges for internal and terminal nodes using the *stub operator* $\hat{\mathfrak{r}}_j$ (23) together with Eq. (26) and Eq. (27)

$$\check{\mathfrak{a}}_j = \hat{\mathfrak{r}}_j\,\frac{\hat{\sigma}^x_j\hat{\sigma}^z_{2j} + \imath\hat{\sigma}^y_j\hat{\sigma}^z_{2j+1}}{2} = \hat{\mathfrak{r}}_j\hat{a}_{j\triangleleft 2j}, \quad j = 1,\ldots,2^{\mathsf{L}-1}-1, \quad (54a)$$

$$\check{\mathfrak{a}}_j = \hat{\mathfrak{r}}_j\,\frac{\hat{\sigma}^x_j + \imath\hat{\sigma}^y_j}{2} = \hat{\mathfrak{r}}_j\hat{a}_j, \quad j = 2^{\mathsf{L}-1},\ldots,2^{\mathsf{L}}-1, \quad (54b)$$

where $\hat{a}_{j\triangleleft 2j}$ is generalization of the conditional operator (53) with index j 'controlled' by the pair $2j, 2j+1$

$$\begin{aligned}\hat{a}_{j\triangleleft 2j} &\doteq \frac{\hat{\sigma}^x_j\hat{\sigma}^z_{2j} + \imath\hat{\sigma}^y_j\hat{\sigma}^z_{2j+1}}{2}\\ &= \hat{a}_j(\hat{n}^0_{2j}\hat{n}^0_{2j+1} - \hat{n}_{2j}\hat{n}_{2j+1})\\ &\quad + \hat{a}^\dagger_j(\hat{n}^0_{2j}\hat{n}_{2j+1} - \hat{n}_{2j}\hat{n}^0_{2j+1}).\end{aligned} \quad (55)$$

An example for $\mathsf{L} = 4$ is depicted in Fig. 6. The constructions of $\check{\mathfrak{a}}_j$, $\check{\mathfrak{a}}^\dagger_j$ include three different nodes for $j = 1,\ldots,7$ and only one node for $j = 8,\ldots,15$.

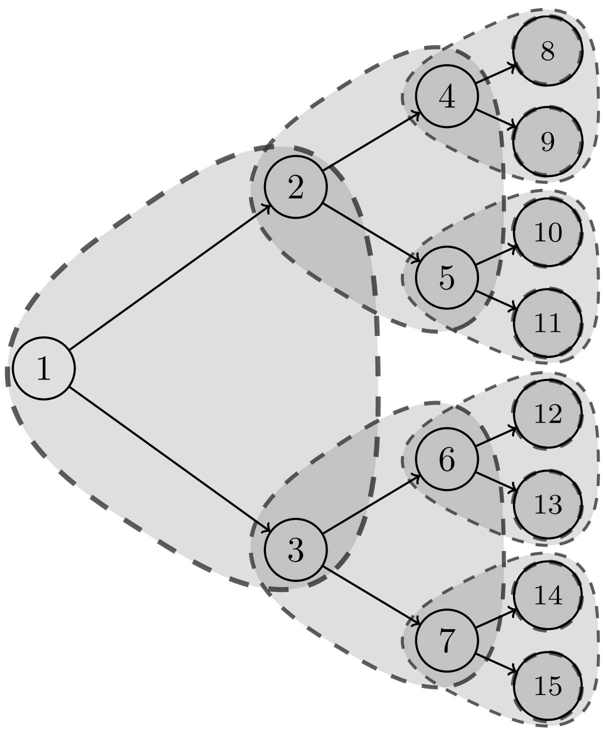

Figure 6: *Nodes groups for* $\check{\mathfrak{a}}_j$, $\check{\mathfrak{a}}^\dagger_j$ *in binary tree.*

Let us now consider analogues of Eq. (39)

$$\check{\Sigma}_{j,k} = \frac{\check{\mathfrak{a}}^\dagger_j\check{\mathfrak{a}}_k + \check{\mathfrak{a}}^\dagger_k\check{\mathfrak{a}}_j}{2}, \quad \check{\Lambda}_{j,k} = \frac{\check{\mathfrak{a}}^\dagger_j\check{\mathfrak{a}}_k - \check{\mathfrak{a}}^\dagger_k\check{\mathfrak{a}}_j}{2\imath}. \quad (56)$$

and Eq. (42) for *modified number (of 'particles') operator*

$$\check{\mathcal{N}} = \sum_{k=1}^{m} \check{\mathfrak{a}}_k^\dagger \check{\mathfrak{a}}_k = \sum_{k=1}^{m} \check{\mathfrak{n}}_k, \tag{57}$$

where $\check{\mathfrak{n}}_k = \check{\mathfrak{a}}_k^\dagger \check{\mathfrak{a}}_k$ are *modified 'occupation number' operators*.

The 'vacuum state' (40) for a binary tree also satisfies $\check{\mathfrak{a}}_j|\varnothing\rangle = 0$ for any j. It is clear that for terminal nodes $j \geq 2^{\mathsf{L}-1}$, because the tensor product for $\check{\mathfrak{a}}_j$ includes $\hat{a}_j$ (54b). For alternative expression with three nodes Eq. (54a) the controlled terms $\hat{a}_{j \triangleleft 2j}$ (55) for $|\varnothing\rangle$ also act as annihilation operator on qubit j, because the two 'control qubits' $2j$ and $2j+1$ are zeros, *cf* Eq. (53).

Thus, operators (42) also satisfy the condition $\check{\Sigma}_{j,k}|\varnothing\rangle = \check{\Lambda}_{j,k}|\varnothing\rangle = 0$ and the same is true for Hamiltonians represented as linear combination of the operators, $\check{\mathcal{H}}|\varnothing\rangle = 0$. Quantum gates and circuits generated with such Hamiltonians

$$\check{\mathcal{U}} = \exp(-\imath\check{\mathcal{H}}\tau) \tag{58}$$

do not change the 'vacuum state' $\check{\mathcal{U}}|\varnothing\rangle = |\varnothing\rangle$ similarly to $\hat{\mathcal{U}}$ in Eq. (41), but must commute with the modified operator $\check{\mathcal{N}}$ instead of $\hat{\mathcal{N}}$.

Let us consider analogues of states (44)

$$\begin{aligned} |\check{\Xi}^{(\check{N})}_{j_1 \cdots j_{\check{N}}}\rangle &= \check{\mathfrak{a}}^\dagger_{j_{\check{N}}} \cdots \check{\mathfrak{a}}^\dagger_{j_1}|\varnothing\rangle, \\ \check{\mathcal{N}}|\check{\Xi}^{(\check{N})}_{j_1 \cdots j_{\check{N}}}\rangle &= \check{N}|\check{\Xi}^{(\check{N})}_{j_1 \cdots j_{\check{N}}}\rangle. \end{aligned} \tag{59}$$

Quantum gates defined by Eq. (58) due to the property $\check{\mathcal{N}}\check{\mathcal{U}} = \check{\mathcal{U}}\check{\mathcal{N}}$ do not change $\check{N}$, but the number of units in elements of the computational basis may not be fixed.

Let us consider an example of Eq. (59) with single creation operator

$$|\check{\Xi}^{(1)}_k\rangle = \check{\mathfrak{a}}^\dagger_k|\varnothing\rangle \doteq |\underline{\check{k}}\rangle, \quad \check{\mathcal{N}}|\underline{\check{k}}\rangle = |\underline{\check{k}}\rangle, \quad 1 \leq k \leq m. \tag{60}$$

The operators $\check{\mathfrak{a}}^\dagger_k$ are obtained from $\check{\mathfrak{a}}_k$ (54) by Hermitian conjugation and $|\underline{\check{k}}\rangle$ is up to phase $\imath$ an element of the computational basis with units only in positions corresponding to the 'path' from the root to node k. The number of units is equal to the level ℓ of the node in the tree

$$\hat{\mathcal{N}}^z|\underline{\check{k}}\rangle = \ell_k|\underline{\check{k}}\rangle, \quad \ell_k = \lfloor \log_2 k \rfloor + 1. \tag{61}$$

The eigenvalues of $\check{\mathcal{N}}$ operators Eq. (57) can be expressed directly in the computational basis using an analogue of sums (42) or (47) with operators $\check{\mathfrak{n}}_j$ written for different ranges using Eq. (54)

$$\check{\mathfrak{n}}_j = \check{\mathfrak{a}}_j^\dagger \check{\mathfrak{a}}_j = \frac{\mathbb{1} - \hat{\sigma}^z_j \hat{\sigma}^z_{2j} \hat{\sigma}^z_{2j+1}}{2}, \quad j = 1, \ldots, 2^{\mathsf{L}-1} - 1, \tag{62a}$$

$$\check{\mathfrak{n}}_j = \check{\mathfrak{a}}_j^\dagger \check{\mathfrak{a}}_j = \frac{\mathbb{1} - \hat{\sigma}^z_j}{2}, \quad j = 2^{\mathsf{L}-1}, \ldots, 2^{\mathsf{L}} - 1. \tag{62b}$$

The quadratic expressions $\hat{\mathfrak{h}}$ defined in Eq. (28) may be rewritten using Eq. (29) and Eq. (31)

$$\check{\mathfrak{n}}_j = \frac{\mathbb{1} - \hat{\mathfrak{h}}^z_j}{2}, \quad j = 1, \ldots, 2^{\mathsf{L}} - 1. \tag{63}$$

The tensor product of $\hat{\sigma}^z$ is built up from diagonal matrices and the eigenvalues η_j of $\hat{\mathfrak{h}}^z_j$ (31) for eigenvectors from the computational basis can be expressed as

$$\begin{aligned} \hat{\mathfrak{h}}^z_j|n_1, \ldots, n_m\rangle &= \eta_j|n_1, \ldots, n_m\rangle, \\ \eta_j &= (-1)^{n_j + n_{2j} + n_{2j+1}} \quad (j < 2^{\mathsf{L}-1}) \end{aligned} \tag{64}$$

and due to simple identity

$$\frac{1 - (-1)^k}{2} = k \bmod 2$$

eigenvalues of $\check{\mathfrak{n}}_j$ using Eq. (62) and Eq. (64) can be expressed as

$$\check{n}_j = \begin{cases} n_j \oplus n_{2j} \oplus n_{2j+1}, & j = 1, \ldots, 2^{\mathsf{L}-1} - 1, \\ n_j, & j = 2^{\mathsf{L}-1}, \ldots, 2^{\mathsf{L}} - 1, \end{cases} \tag{65}$$

where $\oplus$ denotes XOR (exclusive OR) operation for binary values

$$\check{n}_j = n_j \oplus n_{2j} \oplus n_{2j+1} = (n_j + n_{2j} + n_{2j+1}) \bmod 2. \tag{66}$$

The eigenvalue of $\check{\mathcal{N}}$ is

$$\check{N} = \sum_{j=1}^{m} \check{n}_j. \tag{67}$$

Let us consider an example with single creation operator for node k (60). The positions of units produce some path from the root to k. Any triple of nodes in Eq. (65) for $j \neq k$ contains zero or two units and $\check{n}_j$ is the only nonzero element in sum (67), $\check{n}_j = \delta_{jk}$, thus, $\check{N} = 1$.

Let us consider m elements with a single unit in the computational basis. The method used above illustrates that $\check{N} = 1$ only for $j = 1$, but $\check{N} = 2$ for $j > 1$ due to second unit in sum (67), because the triple for $k = j \operatorname{div} 2$ in Eq. (65) also contains node j. It may be also checked directly, that for given indexing (26)

$$\begin{aligned} |\check{\Xi}^{(2)}_{j',j}\rangle = \check{\mathfrak{a}}^\dagger_j \check{\mathfrak{a}}^\dagger_{j'}|\varnothing\rangle, \quad j &= 2, \ldots, m = 2^{\mathsf{L}} - 1, \\ j' &= j \operatorname{div} 2 \end{aligned} \tag{68}$$

is an element of the computational basis (up to $\imath$) with single unit in position j, see Eq. (49)

$$|\check{\Xi}^{(2)}_{j \div 2, j}\rangle = \check{\mathfrak{a}}^\dagger_j \check{\mathfrak{a}}^\dagger_{j \div 2}|\varnothing\rangle = \imath|\underline{j}\rangle, \quad j = 2, \ldots, m, \tag{69}$$

where the notation $j \div 2 = j \operatorname{div} 2$ is used for brevity and both elements in each pair $j \in \{2j', 2j'+1\}$ are taken into account for $j > 1$. Thus

$$\check{\mathcal{N}}|\underline{1}\rangle = |\underline{1}\rangle, \quad \check{\mathcal{N}}|\underline{j}\rangle = 2|\underline{j}\rangle, \qquad j > 1. \tag{70}$$

However, elements of the computational basis with units in both positions $2j'$ and $2j'+1$ also may be expressed in similar way

$$|\check{\Xi}^{(2)}_{2j',2j'+1}\rangle = \check{\mathfrak{a}}^\dagger_{2j'+1}\check{\mathfrak{a}}^\dagger_{2j'}|\varnothing\rangle = |\underline{2j',2j'+1}\rangle, \quad j' = 1,\ldots,2^{\mathsf{L}-1}-1, \tag{71}$$

where the notation from Ref. [1] is used

$$|\underline{k,k+1}\rangle = |\underbrace{0\ldots0}_{k-1}11\underbrace{0\ldots0}_{m-k-2}\rangle. \tag{72}$$

Thus, such states also belong to subspace corresponding to eigenvalue 2 of the operator $\check{\mathcal{N}}$, *cf* Eq. (70)

$$\check{\mathcal{N}}|\underline{2j,2j+1}\rangle = 2|\underline{2j,2j+1}\rangle, \quad 1 \le j \le 2^{\mathsf{L}-1}-1. \tag{73}$$

Let us recollect that quantum circuits with gates generated by Hamiltonian (58) can be used for transformation between different states from subspaces with *the same* eigenvalue of $\check{\mathcal{N}}$.

6 Efficient simulation

Let us start with analogues of efficient classical simulation considered in Ref. [22, 23] with calculation of expectation values of generators $\check{\mathfrak{e}}_j$ for binary trees using the exponential representation of gates $\check{U}$ with 'quadratic' Hamiltonian $\check{H}$ (32).

Unitary operators $\pm\check{U}_{\mathsf{R}} \in \mathrm{SU}(2^m)$ (elements of the Spin group) are corresponding to orthogonal matrix R with the property

$$\check{U}_{\mathsf{R}}\check{\mathfrak{e}}_j\check{U}^\dagger_{\mathsf{R}} = \sum_k \mathsf{R}_{kj}\check{\mathfrak{e}}_k, \tag{74}$$

where the summation is applied to the actually used set of indices. For a binary tree, natural choice may include either $k = 1,\ldots,2m+1$ for $\mathcal{C}\ell(2m+1)$, $\mathrm{Spin}(2m+1)$ and $\mathsf{R} \in \mathrm{SO}(2m+1)$ or $k = 2,\ldots,2m+1$ for $\mathcal{C}\ell(2m)$, $\mathrm{Spin}(2m)$ and $\mathsf{R} \in \mathrm{SO}(2m) \subset \mathrm{SO}(2m+1)$, *cf* Eq. (27) for $m = 3$.

Here, consideration of all generators with $\mathsf{R} \in \mathrm{SO}(2m+1)$ may be useful, because $\check{\mathfrak{e}}_1$ appears in the quadratic Hamiltonian in terms for links such as $\hat{\mathfrak{h}}^x_1$, $\hat{\mathfrak{h}}^y_1$ in Eq. (30). However, $\check{\mathfrak{e}}_1$ is dropped in constructions with creation and annihilation operators (50).

The evolution of state due to such unitary operators is $|\phi'\rangle = \check{U}_{\mathsf{R}}|\phi\rangle$ and the expectation value of $\check{\mathfrak{e}}_j$ is

$$\langle\phi'|\check{\mathfrak{e}}_j|\phi'\rangle = \langle\phi|\check{U}^\dagger_{\mathsf{R}}\check{\mathfrak{e}}_j\check{U}_{\mathsf{R}}|\phi\rangle = \sum_k \mathsf{R}_{jk}\langle\phi|\check{\mathfrak{e}}_k|\phi\rangle, \tag{75}$$

where the order of indices is changed in comparison with Eq. (74) due to inversion $\check{U}^\dagger_{\mathsf{R}} = \check{U}^{-1}_{\mathsf{R}}$. Eq. (75) is the formal algebraic analogue of an equation for matchgates [22] with $\mathsf{R} \in \mathrm{SO}(2m)$, but for the different operators $\check{U}_{\mathsf{R}}$, $\check{\mathfrak{e}}_j$ are constructed using binary trees instead of linear chains. The quadratic terms were more suitable in Ref. [22, 23] and analogues of such expressions also can be introduced

$$\begin{aligned}\langle\phi'|\imath\check{\mathfrak{e}}_{j_1}\check{\mathfrak{e}}_{j_2}|\phi'\rangle &= \langle\phi|\imath\check{U}^\dagger_{\mathsf{R}}\check{\mathfrak{e}}_{j_1}\check{\mathfrak{e}}_{j_2}\check{U}_{\mathsf{R}}|\phi\rangle \\ &= \langle\phi|\imath(\check{U}^\dagger_{\mathsf{R}}\check{\mathfrak{e}}_{j_1}\check{U}_{\mathsf{R}})(\check{U}^\dagger_{\mathsf{R}}\check{\mathfrak{e}}_{j_2}\check{U}_{\mathsf{R}})|\phi\rangle \\ &= \sum_{k_1\neq k_2}\mathsf{R}_{k_1j_1}\mathsf{R}_{k_2j_2}\langle\phi|\imath\check{\mathfrak{e}}_{k_1}\check{\mathfrak{e}}_{k_2}|\phi\rangle,\end{aligned} \tag{76}$$

where the condition $k_1 \neq k_2$ can be used because the terms with equal indices disappear due to orthogonality of matrix R.

For *terminal* indices $j = 2^{\mathsf{L}-1},\ldots,2^{\mathsf{L}}-1$ quadratic terms $\imath\check{\mathfrak{e}}_{2j}\check{\mathfrak{e}}_{2j+1} = \hat{\mathfrak{h}}^z_j$ (28) are equal with single Pauli matrix $\hat{\sigma}^z_j$ (29) and the expectation value is analogous to Ref. [22, 23]. However, for *internal* indices $j = 1,\ldots,2^{\mathsf{L}-1}-1$, $\hat{\mathfrak{h}}^z_j$ are product of three Pauli matrices (31). The latter may be written

$$\langle\phi|\imath\check{\mathfrak{e}}_{2j}\check{\mathfrak{e}}_{2j+1}|\phi\rangle = \begin{cases}\langle\phi|\hat{\sigma}^z_j\hat{\sigma}^z_{2j}\hat{\sigma}^z_{2j+1}|\phi\rangle, \\ \qquad j = 1,\ldots,2^{\mathsf{L}-1}-1 \\ \langle\phi|\hat{\sigma}^z_j|\phi\rangle, \\ \qquad j = 2^{\mathsf{L}-1},\ldots,2^{\mathsf{L}}-1\end{cases}. \tag{77}$$

Using the definition of $\check{\mathfrak{n}}_j$ (63), it may be rewritten in agreement with analogous equation for $\check{n}_j$ (65)

$$\langle\phi|\check{\mathfrak{n}}_j|\phi\rangle = \langle\check{n}_j\rangle = \begin{cases}\langle n_j \oplus n_{2j} \oplus n_{2j+1}\rangle, \\ \qquad j = 1,\ldots,2^{\mathsf{L}-1}-1 \\ \langle n_j\rangle, \quad j = 2^{\mathsf{L}-1},\ldots,2^{\mathsf{L}}-1\end{cases}, \tag{78}$$

where the standard notation $\langle\cdots\rangle$ for expectation value is used, *e.g.*, $\langle n_j\rangle = p_{1\,j}$ is the probability to measure value 1 for qubit j.

For the terminal nodes $j = 2^{\mathsf{L}-1},\ldots,2^{\mathsf{L}}-1$, the result of qubit measurement in the computational basis $n_j = \check{n}_j$ can be directly found from Eq. (76). For the previous level $\ell_j = \mathsf{L}-1$ with indices $j = 2^{\mathsf{L}-2},\ldots,2^{\mathsf{L}-1}-1$, it includes an expression with three terms

$$n_j = \check{n}_j \oplus n_{2j} \oplus n_{2j+1} = \check{n}_j \oplus \check{n}_{2j} \oplus \check{n}_{2j+1},$$

for level $\ell_j = \mathsf{L}-2$, the expression n via $\check{n}$ requires seven terms

$$n_j = \check{n}_j \oplus \check{n}_{2j} \oplus \check{n}_{4j} \oplus \check{n}_{4j+1} \oplus \check{n}_{2j+1} \oplus \check{n}_{4j+2} \oplus \check{n}_{4j+3}.$$

For deeper levels $\ell_j = \mathsf{L} - d$, similar expansions produce $2^{d+1} - 1$ terms

$$n_j = \begin{cases} \Big(\check{n}_j + \sum\limits_{k\in d(j)} \check{n}_k\Big) \bmod 2, \\ \qquad\qquad j = 1,\ldots,2^{\mathsf{L}-1}-1 \\ \\ \check{n}_j, \quad j = 2^{\mathsf{L}-1},\ldots,2^{\mathsf{L}}-1 \end{cases}, \tag{79}$$

where $d(j)$ are *all descendants* of node j, or, more briefly

$$n_j = \sum_{k\in s(j)} \check{n}_k \mod 2. \tag{79$'$}$$

where $s(j) = d(j) \cup \{j\}$ are all nodes of the subtree with root j, including the trivial case with a single term $s(j) = \{j\}$ for terminal qubit nodes.

Thus, the analogue of the approach used in Ref. [22,23] can be applied only either to computation of $\langle\check{n}_j\rangle$ or for measurements of separate qubits in terminal nodes.

For internal nodes with level $\ell < \mathsf{L}$, even for a single qubit measurement outcome should be used more complicated approach such as the one applied to multi-qubit outputs in a standard case [24], but with measurement of $2^{\mathsf{L}-l}$ quantum 'binary variables' $\check{n}_j$ expressed as XOR operations with qubit values. Thus, despite of some resemblance with matchgate circuits, the effective modeling with binary trees deserves special consideration.

Together with possible difficulties for internal nodes, it has specific advantages for terminal qubits. Linear combinations of quadratic Hamiltonians (29) may generate arbitrary rotation and the expectation values $\langle Z_j\rangle$ in the computational basis (77) can be extended for efficient simulation of qubit measurement 'along any axis.'

A pair of terminal qubits with indices $2j, 2j+1$ have common parent $j = 2^{\mathsf{L}-2},\ldots,2^{\mathsf{L}-1}-1$. Let us show, that for parent qubit fixed in state $|0\rangle$ any transformation from SU(4) group may be implemented using only quadratic Hamiltonian. The construction with auxiliary qubit uses isomorphism between SU(4) and Spin(6) and is similar to the method discussed in Ref. [25].

Let us extend a simpler example $\mathsf{L} = 2$, $m = 3$ (27) to write seven generators associated with the 'terminal triple' of qubits with parent node $2^{\mathsf{L}-2} \le j < 2^{\mathsf{L}-1}$ for arbitrary $\mathsf{L} \ge 2$

$$\begin{aligned} \check{\mathfrak{e}}_j = \hat{\mathfrak{r}}_j\hat{\sigma}^z_j, \qquad \check{\mathfrak{e}}_{2j} &= \hat{\mathfrak{r}}_j\hat{\sigma}^x_j\hat{\sigma}^z_{2j}, & \check{\mathfrak{e}}_{2j+1} &= \hat{\mathfrak{r}}_j\hat{\sigma}^y_j\hat{\sigma}^z_{2j+1}, \\ \check{\mathfrak{e}}_{4j} &= \hat{\mathfrak{r}}_j\hat{\sigma}^x_j\hat{\sigma}^x_{2j}, & \check{\mathfrak{e}}_{4j+2} &= \hat{\mathfrak{r}}_j\hat{\sigma}^y_j\hat{\sigma}^x_{2j+1}, \\ \check{\mathfrak{e}}_{4j+1} &= \hat{\mathfrak{r}}_j\hat{\sigma}^x_j\hat{\sigma}^y_{2j}, & \check{\mathfrak{e}}_{4j+3} &= \hat{\mathfrak{r}}_j\hat{\sigma}^y_j\hat{\sigma}^y_{2j+1}. \end{aligned} \tag{80}$$

Products of two generators (80) produce 21 different terms, but only 15 of them do not change the parent qubit with state $|0\rangle$

$$\hat{\sigma}^\mu_{2j}, \quad \hat{\sigma}^\nu_{2j+1}, \quad \hat{\sigma}^z_j\hat{\sigma}^\mu_{2j}\hat{\sigma}^\nu_{2j+1}, \qquad \mu,\nu = x,y,z. \tag{81}$$

The linear combinations of analogues of terms (81) without multiplier $\hat{\sigma}^z_j$ would produce arbitrary traceless Hamiltonian for two qubits, but $\hat{\sigma}^z$ acts as identity on state $|0\rangle$ and so terms (81) also may generate arbitrary SU(4) transformation of two terminal qubits if the common parent qubit is $|0\rangle$. □

Let us now consider construction of gates $\check{\mathcal{U}}$ (58) generated by quadratic combinations (56) of ladder operators $\check{\mathfrak{a}}_j$ and $\check{\mathfrak{a}}^\dagger_k$ (50) for a binary tree. For this case, instead of Eq. (74) an auxiliary matrix $\mathsf{U} \in \mathrm{SU}(m)$ can be introduced for operators $\pm\check{\mathcal{U}}_{\mathsf{U}} \in \mathrm{SU}(2^m)$ with formal analogue of well-known relations for ladder operators [1,16]

$$\check{\mathcal{U}}_{\mathsf{U}}\check{\mathfrak{a}}_k\check{\mathcal{U}}^\dagger_{\mathsf{U}} = \sum_{j=1}^m \bar{\mathsf{U}}_{kj}\check{\mathfrak{a}}_j, \quad \check{\mathcal{U}}_{\mathsf{U}}\check{\mathfrak{a}}^\dagger_k\check{\mathcal{U}}^\dagger_{\mathsf{U}} = \sum_{j=1}^m \mathsf{U}^\dagger_{jk}\check{\mathfrak{a}}^\dagger_j, \tag{82}$$

where $\bar{\mathsf{U}}_{kj}$ is complex conjugation of coefficients and $\mathsf{U}^\dagger = \mathsf{U}^{-1}$ for unitary matrix U.

A 'path-state' $|\underline{\check{k}}\rangle$ (60) satisfies an analogue of equations used in Ref. [1] for $|\underline{k}\rangle$ defined by Eq. (48) up to trivial change of variables, *i.e.*,

$$\begin{aligned} \check{\mathcal{U}}_{\mathsf{U}}|\underline{\check{k}}\rangle &= \check{\mathcal{U}}_{\mathsf{U}}\check{\mathfrak{a}}^\dagger_k|\varnothing\rangle = \check{\mathcal{U}}_{\mathsf{U}}\check{\mathfrak{a}}^\dagger_k\check{\mathcal{U}}^\dagger_{\mathsf{U}}|\varnothing\rangle \\ &= \sum_{l=1}^m \mathsf{U}^\dagger_{lk}\check{\mathfrak{a}}^\dagger_l|\varnothing\rangle = \sum_{l=1}^m \mathsf{U}^\dagger_{lk}|\underline{\check{l}}\rangle. \end{aligned} \tag{83}$$

Let us consider linear superposition of path states $|\underline{\check{\chi}}\rangle = \sum_{k=1}^m \chi_k|\underline{\check{k}}\rangle$

$$\begin{aligned} \check{\mathcal{U}}_{\mathsf{U}}|\underline{\check{\chi}}\rangle &= \check{\mathcal{U}}_{\mathsf{U}}\sum_{k=1}^m \chi_k|\underline{\check{k}}\rangle = \sum_{l,k=1}^m \mathsf{U}^\dagger_{lk}\chi_k|\underline{\check{l}}\rangle \equiv \sum_{l=1}^m \chi'_l|\underline{\check{l}}\rangle, \\ \chi'_l &\doteq \sum_{k=1}^m \mathsf{U}^\dagger_{lk}\chi_k. \end{aligned} \tag{84}$$

Eq. (84) for 'single-path' states ($\check{N} = 1$) is similar to the evolution of 'single-particle' case ($N^z = 1$) for *qubit chain* [1], but for all nodes except of the root in *binary qubit tree*, $|\underline{k}\rangle$ belongs to $\check{N} = 2$ subspace due to Eq. (70). However, the same subspace also includes pairs $|\underline{2j, 2j+1}\rangle$ (70) and an analogy with 'two-particle' case is also relevant.

For Hamiltonians respecting $\hat{N}$ or $\check{N}$, the consideration of 'number-preserving' subspaces is natural for models of state transfer in quantum chains [1,26] or trees. The two-qubit state can be decomposed into three parts:

$$|\psi\rangle = \underbrace{\overbrace{c_{00}|00\rangle}^{N=0}}_{\check{N}=0} + \underbrace{\overbrace{c_{01}|01\rangle + c_{10}|10\rangle}^{N=1} + \overbrace{c_{11}|11\rangle}^{N=2}}_{\check{N}=2}, \tag{85}$$

but terms with $N = 1$ and $N = 2$ in Eq. (85) in the binary tree for pairs of nodes $2j, 2j+1$ ($0 < j < 2^{\mathsf{L}-1}$) belong to the same subspace $\check{N} = 2$, and, furthermore, $N = \check{N} = 0$ is not affected by $\check{\mathcal{U}}$ (58) for state transfer.

For two consequent indices $2j, 2j+1$, three terms with $N \neq 0$ ($\check{N} = 2$) in Eq. (85) are generated by application to $|\varnothing\rangle$ of different pairs of operators between the same triple $\breve{\mathfrak{a}}^\dagger_j$, $\breve{\mathfrak{a}}^\dagger_{2j}$ and $\breve{\mathfrak{a}}^\dagger_{2j+1}$ due to Eq. (69) and Eq. (71). Thus, as a result of perfect transfer of such two-qubit pair into new position $2k, 2k+1$ indices by operator $\check{\mathcal{U}}_{\mathsf{U}}$ should correspond to unitary matrix U with simple constrains on three elements

$$|\mathsf{U}_{jk}| = |\mathsf{U}_{2j,2k}| = |\mathsf{U}_{2j+1,2k+1}| = 1. \tag{86}$$

For consideration of perfect transfer with single qubit, one condition in Eq. (86) may be superfluous.

The example illustrates possibility of exponential decrease of model dimension from 2^m to m, but the construction of U with a sequence of steps or appropriate Hamiltonians deserves separate consideration elsewhere. Even the reduced problem is more difficult than analogous example for qubit chain because of less trivial structure of the graph itself and more complicated properties of modified operators such as $\breve{\mathfrak{a}}$ and $\breve{\mathfrak{a}}^\dagger$.

7 General trees

7.1 Alternative encoding of binary trees

In the binary trees discussed earlier, all nodes attached to z-links were deleted. Let us consider as an alternative the binary x-z trees with y-links collapsed instead. The *stub operator* $\hat{\mathfrak{r}}_j$ (19) for such a tree contains $\hat{\sigma}^x$, $\hat{\sigma}^z$ and generators may contain no more than one $\hat{\sigma}^y$.

Some constructions discussed below become more natural, if new root with index zero is attached by x-link. Similar method was briefly mentioned in Section 3 and for Υ_{L}-tree it produces '$\Upsilon^\circ_{\mathsf{L}}$-tree' of height L with 2^{L} nodes. In this case appropriate pairs of generators can be chosen to provide necessary coupling of $\hat{\sigma}_x$ and $\hat{\sigma}_y$ for qubits with the same index for specific construction of ladder operators (33) discussed below, see Fig. 7.

Let us consider an example with eight qubits. Similarly to binary trees discussed earlier, only z-term for root $\hat{\sigma}^z_0$ is excluded from such a coupling and internal nodes require more complicated expressions for ladder operators

$$\breve{\mathfrak{a}}_0 = \frac{\hat{\sigma}^x_0\hat{\sigma}^z_1\hat{\sigma}^z_3\hat{\sigma}^z_7 + \imath\hat{\sigma}^y_0}{2}, \quad \breve{\mathfrak{a}}_1 = \hat{\sigma}^x_0\frac{\hat{\sigma}^x_1\hat{\sigma}^z_2\hat{\sigma}^z_5 + \imath\hat{\sigma}^y_1}{2},$$
$$\breve{\mathfrak{a}}_2 = \hat{\sigma}^x_0\hat{\sigma}^x_1\frac{\hat{\sigma}^x_2\hat{\sigma}^z_4 + \imath\hat{\sigma}^y_2}{2}, \quad \breve{\mathfrak{a}}_3 = \hat{\sigma}^x_0\hat{\sigma}^z_1\frac{\hat{\sigma}^x_3\hat{\sigma}^z_6 + \imath\hat{\sigma}^y_3}{2}, \tag{87a}$$

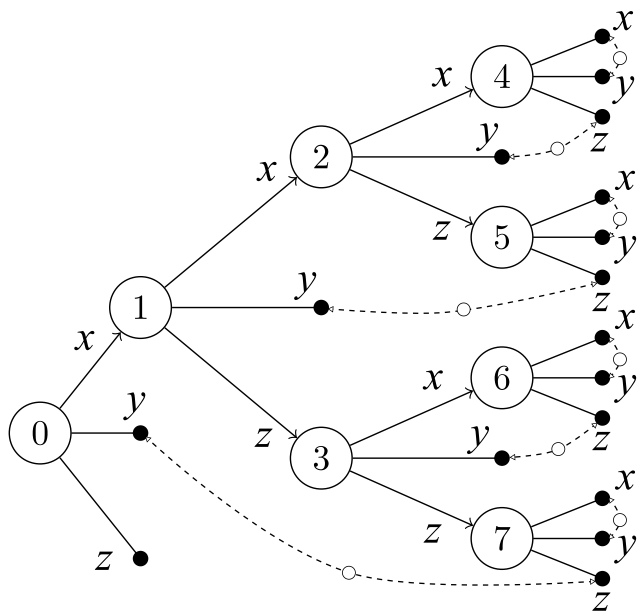

Figure 7: *Pair of nodes in binary* x-z $\Upsilon^\circ_{\mathsf{L}}$*-tree for* $\mathsf{L} = 3$.

in comparison with terminal qubit nodes, *cf* Eq. (54b)

$$\breve{\mathfrak{a}}_4 = \hat{\sigma}^x_0\hat{\sigma}^x_1\hat{\sigma}^x_2\frac{\hat{\sigma}^x_4 + \imath\hat{\sigma}^y_4}{2}, \quad \breve{\mathfrak{a}}_5 = \hat{\sigma}^x_0\hat{\sigma}^x_1\hat{\sigma}^z_2\frac{\hat{\sigma}^x_5 + \imath\hat{\sigma}^y_5}{2},$$
$$\breve{\mathfrak{a}}_6 = \hat{\sigma}^x_0\hat{\sigma}^z_1\hat{\sigma}^x_3\frac{\hat{\sigma}^x_6 + \imath\hat{\sigma}^y_6}{2}, \quad \breve{\mathfrak{a}}_7 = \hat{\sigma}^x_0\hat{\sigma}^x_1\hat{\sigma}^z_3\frac{\hat{\sigma}^x_7 + \imath\hat{\sigma}^y_7}{2}. \tag{87b}$$

In such construction for each terminal node j there are two generators with terms $\hat{\sigma}^x_j$ and $\hat{\sigma}^y_j$ coupled by natural way (87b), but the generator with $\hat{\sigma}^z_j$ is coupled with some internal node j' linked with j by path $xz\cdots z$ in agreement with Eq. (87a), see Fig. 7.

Let us consider the structure of expressions for internal nodes such as Eq. (87a). For some set of nodes ('chain') $c = \{c_1, \ldots, c_l\}$, the following concise notation will be used

$$\hat{\mathfrak{s}}^z_c = \hat{\sigma}^z_{c_1}\cdots\hat{\sigma}^z_{c_l}. \tag{88}$$

Let us also introduce the operators

$$\hat{n}_{\oplus_c} = \frac{\mathbb{1} - \hat{\sigma}^z_{c_1}\cdots\hat{\sigma}^z_{c_l}}{2} = \frac{\mathbb{1} - \hat{\mathfrak{s}}^z_c}{2},$$
$$\hat{n}^0_{\oplus_c} = \mathbb{1} - \hat{n}_{\oplus_c} = \frac{\mathbb{1} + \hat{\mathfrak{s}}^z_c}{2}. \tag{89}$$

Such projectors have eigenvalues expressed as XOR of nodes from set c

$$\hat{n}_{\oplus_c}|n_1, \ldots, n_m\rangle = n_{\oplus_c}|n_1, \ldots, n_m\rangle,$$
$$n_{\oplus_c} = n_{c_1} \oplus \cdots \oplus n_{c_l}. \tag{90}$$

Specific term from the expressions for internal nodes such as Eq. (87a) may be rewritten

$$\begin{aligned}\hat a_{j\oplus_c} &= \frac{\hat\sigma^x_j \hat{\mathfrak{s}}^z_c + \imath\hat\sigma^y_j}{2} \\ &= \frac{\hat\sigma^x_j+\imath\hat\sigma^y_j}{2}\cdot\frac{\hat{\mathfrak{s}}^z_c+\mathbb{1}}{2} + \frac{\hat\sigma^x_j-\imath\hat\sigma^y_j}{2}\cdot\frac{\hat{\mathfrak{s}}^z_c-\mathbb{1}}{2} \\ &= \hat a_j\frac{\mathbb{1}+\hat{\mathfrak{s}}^z_c}{2} - \hat a_j^\dagger\frac{\mathbb{1}-\hat{\mathfrak{s}}^z_c}{2} = \hat a_j \hat n^0_{\oplus_c} - \hat a^\dagger_j \hat n_{\oplus_c}.\end{aligned} \tag{91}$$

Such a term is an analogue of conditional ladder operator (53), because $\hat a_{j\oplus_c}$ is also controlled by few nodes $c_1,\ldots,c_l \in c$.

The analogue of Eq. (54) can be written for binary x-z $\Upsilon^\circ_{\mathsf{L}}$-tree with 2^{L} nodes taking into account the new root with index zero, see Fig. 7

$$\breve{\mathfrak{a}}_j = \hat{\mathfrak{r}}_j \frac{\hat\sigma^x_j \hat{\mathfrak{s}}^z_{c(j)} + \imath\hat\sigma^y_j}{2} = \hat{\mathfrak{r}}_j \hat a_{j\oplus_{c(j)}}, \quad j = 0,\ldots,2^{\mathsf{L}-1}-1, \tag{92a}$$

$$\breve{\mathfrak{a}}_j = \hat{\mathfrak{r}}_j \frac{\hat\sigma^x_j + \imath\hat\sigma^y_j}{2} = \hat{\mathfrak{r}}_j \hat a_j, \quad j = 2^{\mathsf{L}-1},\ldots,2^{\mathsf{L}}-1, \tag{92b}$$

where $\hat{\mathfrak{r}}_j$ is *stub operator* already introduced earlier, *cf* Eq. (92) for $\mathsf{L} = 3$ with Eq. (87). The index $c(j)$ in Eq. (92) denotes set of nodes $c_1,\ldots,c_l$ attached to given node j via chain of z links.

The generators of Clifford algebra for Eq. (92) in agreement with Eq. (38) can be written as

$$\breve{\mathfrak{e}}'_j = \imath\hat{\mathfrak{r}}_j\hat\sigma^x_j\hat{\mathfrak{s}}^z_{c(j)}, \quad \breve{\mathfrak{e}}''_j = \imath\hat{\mathfrak{r}}_j\hat\sigma^y_j, \qquad j \notin \mathcal{T}, \tag{93a}$$

$$\breve{\mathfrak{e}}'_j = \imath\hat{\mathfrak{r}}_j\hat\sigma^x_j, \quad \breve{\mathfrak{e}}''_j = \imath\hat{\mathfrak{r}}_j\hat\sigma^y_j, \qquad j \in \mathcal{T}. \tag{93b}$$

where $\mathcal{T}$ denotes set of terminal nodes, *e.g.*, $j = 2^{\mathsf{L}-1},\ldots,2^{\mathsf{L}}-1$ for trees used in the examples above.

The analogues of Eq. (62) for quadratic operators are also straightforward

$$\breve{\mathfrak{n}}_j = \breve{\mathfrak{a}}^\dagger_j\breve{\mathfrak{a}}_j = \frac{\mathbb{1}-\hat\sigma^z_j\hat{\mathfrak{s}}^z_{c(j)}}{2}, \quad j \notin \mathcal{T}, \tag{94a}$$

$$\breve{\mathfrak{n}}_j = \breve{\mathfrak{a}}^\dagger_j\breve{\mathfrak{a}}_j = \frac{\mathbb{1}-\hat\sigma^z_j}{2}, \quad j \in \mathcal{T}. \tag{94b}$$

The particular example with 2^{L} nodes is interesting due to direct relation with Bravyi–Kitaev (BK) transformation discussed below in Section 7.2, but binary x-z tree also can be used to represent a general tree (g-tree). A node j with l children $c_1,\ldots,c_l$ of such a g-tree should be mapped into node j of binary x-z tree with x-link to only one child node c_1 together with chain of nodes $c_1,\ldots,c_l$ connected by z-links, see Fig. 8. For construction of ladder operators the last node c_l is coupled with node j, *cf* Eq. (87a).

Such construction has some properties of the formalism used earlier due to certain similarity of Eq. (54) and Eq. (62) for binary x-y trees with Eq. (92) and Eq. (94) for nodes with arbitrary number of children obtained from binary x-z trees using the correspondence depicted in Fig. 8.

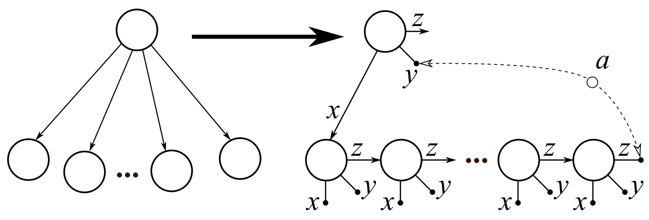

Figure 8: *Multiple children encoding.*

An analogue of Eq. (65) is

$$\breve n_j = \begin{cases} n_j \oplus n_{c_1} \oplus \cdots \oplus n_{c_l}, & j \notin \mathcal{T}, \\ n_j, & j \in \mathcal{T}, \end{cases} \tag{95}$$

where $c_1,\ldots,c_l \in c(j)$ are indices used in $\hat{\mathfrak{s}}^z_{c(j)}$ from Eq. (94a). It is a chain of z-linked nodes in node j of initial binary x-z tree and the same indices correspond to l children of node j in the g-tree obtained by construction depicted in Fig. 8.

Inverse relation for Eq. (95) is similar to Eq. (79) used earlier for binary x-y trees and may be written as

$$n_j = \Big(\breve n_j + \sum_{k\in D(j)} \breve n_k\Big) \bmod 2, \tag{96}$$

where $D(j)$ is (possibly empty) set of all descendants of node j for g-tree obtained from binary x-z tree. The set of nodes $D(j)$ may differs from $d(j)$ for corresponding binary x-z tree, because z-link to 'peers' should not be included in $D(j)$, *e.g.*, in Fig. 9 below $D(3) = \{0,1,2\}$, but $d(3) = \{0,1,2,4,5,6\}$.

7.2 Bravyi–Kitaev transformation

Let us compare the structure of ladder operators (92) or generators (93) with analogous constructions used in Bravyi–Kitaev transformation based on Fenwick trees, see Ref. [9] and some earlier works [27, 28]. The analogues of operators (93) with notation used in Ref. [9] are

$$\begin{aligned}\hat c_j &= \hat Z_{P(j)}\hat X_j \hat X_{U(j)}, \\ \hat d_j &= \hat Z_{C(j)}\hat Y_j \hat X_{U(j)} = \hat Z_{P(j)\setminus F(j)}\hat Y_j \hat X_{U(j)}\end{aligned} \tag{97}$$

where $\hat X$, $\hat Y$, $\hat Z$ denote either Pauli matrices or theirs products similar to Eq. (88), where $U(j)$, $C(j)$, $F(j)$ and $P(j) = C(j) \cup F(j)$ are some set of indices. It can be rewritten to provide similarity with notations used here

$$\breve{\mathfrak{e}}'_j = \imath\hat{\mathfrak{s}}^z_{P(j)}\hat\sigma^x_j\hat{\mathfrak{s}}^x_{U(j)}, \quad \breve{\mathfrak{e}}''_j = \imath\hat{\mathfrak{s}}^z_{C(j)}\hat\sigma^y_j\hat{\mathfrak{s}}^x_{U(j)}, \tag{98}$$

where an analogue of Eq. (88) is used for given set of indices $S(j)$ and Pauli matrix

$$\hat{\mathfrak{s}}^{\mu}_{S} = \prod_{s \in S} \hat{\sigma}^{\mu}_{s}. \tag{88′}$$

Thus, the operator (97) from Ref. [9] corresponds to Eq. (93) if $c(j)$ is denoted as $F(j)$ and the *stub* operator is expressed as

$$\hat{\mathfrak{r}}_j = \pm \hat{\mathfrak{s}}^{z}_{C(j)} \hat{\mathfrak{s}}^{x}_{U(j)}. \tag{99}$$

Let us again consider the example with eight qubits. The indices of nodes in binary x-z trees should be changed to conform to the standard numeration in Bravyi–Kitaev transformation also used in Ref. [9], *cf* Fig. 7 and Fig. 9

	0	1	2	3	4	5	6	7
BK	7	3	1	5	0	2	4	6

(100)

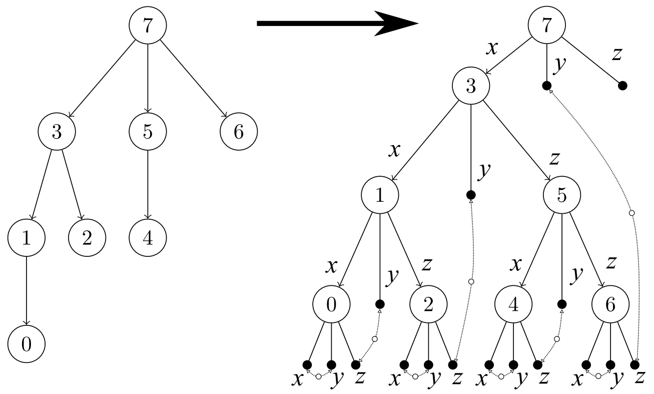

Figure 9: Representation of tree used in Bravyi–Kitaev transformation as binary x-z *tree.*

Ladder operators up to numeration (100) coincide with Eq. (87) for internal nodes

$$\begin{aligned}
\breve{\mathfrak{a}}_1 &= \hat{\sigma}^x_7\hat{\sigma}^x_3(\hat{\sigma}^x_1\hat{\sigma}^z_0 + \imath\hat{\sigma}^y_1)/2,\\
\breve{\mathfrak{a}}_3 &= \hat{\sigma}^x_7(\hat{\sigma}^x_3\hat{\sigma}^z_5\hat{\sigma}^z_4 + \imath\hat{\sigma}^y_3)/2,\\
\breve{\mathfrak{a}}_5 &= \hat{\sigma}^x_7\hat{\sigma}^z_3(\hat{\sigma}^x_1\hat{\sigma}^z_2 + \imath\hat{\sigma}^y_1)/2,\\
\breve{\mathfrak{a}}_7 &= (\hat{\sigma}^x_7\hat{\sigma}^z_3\hat{\sigma}^z_1\hat{\sigma}^z_0 + \imath\hat{\sigma}^y_7)/2
\end{aligned} \tag{101a}$$

and external nodes, respectively

$$\begin{aligned}
\breve{\mathfrak{a}}_0 &= \hat{\sigma}^x_7\hat{\sigma}^x_3\hat{\sigma}^x_1(\hat{\sigma}^x_0 + \imath\hat{\sigma}^y_0)/2,\\
\breve{\mathfrak{a}}_2 &= \hat{\sigma}^x_7\hat{\sigma}^x_3\hat{\sigma}^z_1(\hat{\sigma}^x_2 + \imath\hat{\sigma}^y_2)/2,\\
\breve{\mathfrak{a}}_4 &= \hat{\sigma}^x_7\hat{\sigma}^z_3\hat{\sigma}^x_5(\hat{\sigma}^x_4 + \imath\hat{\sigma}^y_4)/2,\\
\breve{\mathfrak{a}}_6 &= \hat{\sigma}^x_7\hat{\sigma}^x_3\hat{\sigma}^z_5(\hat{\sigma}^x_6 + \imath\hat{\sigma}^y_6)/2.
\end{aligned} \tag{101b}$$

With the new indexing, Eq. (95) may be rewritten for the eight qubits depicted in Fig. 9

$$\begin{aligned}
&\breve{n}_0 = n_0, \quad \breve{n}_2 = n_2, \quad \breve{n}_4 = n_4, \quad \breve{n}_6 = n_6,\\
&\breve{n}_1 = n_1 \oplus n_0, \qquad \breve{n}_5 = n_5 \oplus n_4,\\
&\breve{n}_3 = n_3 \oplus n_1 \oplus n_2, \quad \breve{n}_7 = n_7 \oplus n_3 \oplus n_5 \oplus n_6.
\end{aligned} \tag{102}$$

The inverse relations (96) are

$$\begin{aligned}
&n_0 = \breve{n}_0, \quad n_2 = \breve{n}_2, \quad n_4 = \breve{n}_4, \quad n_6 = \breve{n}_6,\\
&n_1 = \breve{n}_1 \oplus \breve{n}_0, \qquad n_5 = \breve{n}_5 \oplus \breve{n}_4,\\
&n_3 = \breve{n}_0 \oplus \breve{n}_1 \oplus \breve{n}_2 \oplus \breve{n}_3,\\
&n_7 = \breve{n}_0 \oplus \breve{n}_1 \oplus \breve{n}_2 \oplus \breve{n}_3 \oplus \breve{n}_4 \oplus \breve{n}_5 \oplus \breve{n}_6 \oplus \breve{n}_7.
\end{aligned} \tag{103}$$

Let us recollect, what n_j corresponds to single qubit with index j, but $\breve{n}_j$ is ‘BK number’ related with set of qubits affected by ‘modified BK creation operator’ $\breve{\mathfrak{a}}^{\dagger}_j$.

In such a way, the set of equations (103) is in agreement with the usual scheme of Bravyi–Kitaev transformation [10] and it corresponds to an example of Fenwick tree with eight nodes considered in Ref. [9] taking into account the correspondence between g-tree and binary x-z tree discussed in Section 7.1.

8 Conclusion

The construction of Clifford algebras associated with some kinds of trees is discussed in this work. Formally, set of generators can be produced by *deterministic finite automaton* obtained as the extension of ternary tree by addition of some formal output nodes. The binary trees can be formally considered as a reduced case of ternary tree where at least one child for each node is omitted, see Fig. 3. In appropriate cases, the trees can also be used for modeling of quantum state transfer along the edges.

The Spin group can be expressed using exponents with linear combination of terms quadratic by generators of Clifford algebra. Such terms correspond to Hamiltonians in quantum mechanics. The trivial case is a chain associated with standard (Jordan–Wigner) generators of Clifford algebra (5). In this case, the quadratic expression for Hamiltonian of a node is $\mathfrak{e}_{2k-1}\mathfrak{e}_{2k}$ and more general terms $\mathfrak{e}_j\mathfrak{e}_k$ represent expressions with Pauli matrices acting on two or more consequent qubit nodes in the tree.

Both for binary and ternary trees the expressions for generators include sequence of nodes from the root to some terminal node. Thus, quadratic expressions represent single node or segment with a sequence between two nodes. However, the number of formal output nodes of *deterministic finite automaton* attached to given qubit is $n_o = 3 - n_c$, where n_c is the number of children for given qubit in the tree. Thus, for ternary trees, an internal qubit node may be missing in such sequence and binary trees with $n_o > 0$ are more preferable for some purposes.

The construction with trees naturally produces odd number of generators, but any one of them can be expressed as product of others. Due to this property, any generator could be dropped, yet a new set with even number of generators may lack the initial symmetry. Anyway, even number of generators decomposed in pairs can be used for the definition of creation and annihilation (ladder) operators (33). Such construction is appropriate for a general ternary tree, but it looks more natural for reduced cases such as binary trees or linear chains.

The generators of Clifford algebra $\mathfrak{e}_j$ in some physical applications can also be treated as creation operators, but particle and antiparticle become equivalent in this case, because $\mathfrak{e}_j^2 = \mathbb{1}$. The quadratic expressions with generators are convenient for modeling of state transfer. For a system with m qubits and Hilbert space with dimension 2^m, the quadratic Hamiltonian produces evolution described by matrices of rotations in a space with dimension only $2m$ due to main property of Spin groups (74).

Section 7 slightly extends the initial scope of this paper about effective modeling and state transfer to show relations with so-called fermion-to-qubit mapping for applications in quantum computers. It is demonstrated in Section 7.1 that a model with general trees often used for such purposes can be obtained from an alternative reduction of the ternary tree illustrated in Fig. 8. The particular example with Bravyi–Kitaev transformation is explained in Section 7.2.

References

[1] A. Y. Vlasov. Effective simulation of state distribution in qubit chains. *Quantum Information Processing* 2018; **17**(10):269. doi:10.1007/s11128-018-2036-1.

[2] P. Jordan, E. Wigner. Über das Paulische äquivalenzverbot. *Zeitschrift für Physik* 1928; **47**(9):631–651. doi:10.1007/bf01331938.

[3] S. Backens, A. Shnirman, Y. Makhlin. Jordan–Wigner transformations for tree structures. *Scientific Reports* 2019; **9**(1):2598. doi:10.1038/s41598-018-38128-8.

[4] A. M. Szczerba. Spins and fermions on arbitrary lattices. *Communications in Mathematical Physics* 1985; **98**(4):513–524. doi:10.1007/BF01209327.

[5] T. Ried. Jordan–Wigner transformations and quantum spin systems on graphs. Ph.D. thesis (2013). https://www.theorie.physik.uni-muenchen.de/TMP/theses/riedthesis.pdf.

[6] M. Steudtner, S. Wehner. Fermion-to-qubit mappings with varying resource requirements for quantum simulation. *New Journal of Physics* 2018; **20**(6):063010. doi:10.1088/1367-2630/aac54f.

[7] M. Steudtner, S. Wehner. Quantum codes for quantum simulation of fermions on a square lattice of qubits. *Physical Review A* 2019; **99**(2):022308. arXiv:1810.02681. doi:10.1103/PhysRevA.99.022308.

[8] Z. Jiang, A. Kalev, W. Mruczkiewicz, H. Neven. Optimal fermion-to-qubit mapping via ternary trees with applications to reduced quantum states learning. *Quantum* 2020; **4**:276. doi:10.22331/q-2020-06-04-276.

[9] V. Havlíček, M. Troyer, J. D. Whitfield. Operator locality in the quantum simulation of fermionic models. *Physical Review A* 2017; **95**(3):032332. arXiv:1701.07072. doi:10.1103/PhysRevA.95.032332.

[10] S. B. Bravyi, A. Y. Kitaev. Fermionic quantum computation. *Annals of Physics* 2002; **298**(1):210–226. arXiv:quant-ph/0003137. doi:10.1006/aphy.2002.6254.

[11] J. E. Gilbert, M. A. M. Murray. Clifford Algebras and Dirac Operators in Harmonic Analysis. Vol. 26 of *Cambridge Studies in Advanced Mathematics*. Cambridge University Press, Cambridge, 1991. doi:10.1017/cbo9780511611582.

[12] I. R. Porteous. Clifford Algebras and the Classical Groups. Vol. 50 of *Cambridge Studies in Advanced Mathematics*. Cambridge University Press, Cambridge, 1995. doi:10.1017/cbo9780511470912.

[13] A. Y. Vlasov. Clifford algebras and universal sets of quantum gates. *Physical Review A* 2001; **63**(5):054302. arXiv:quant-ph/0010071. doi:10.1103/PhysRevA.63.054302.

[14] D. P. DiVincenzo. Two-bit gates are universal for quantum computation. *Physical Review A* 1995; **51**(2):1015–1022. arXiv:cond-mat/9407022. doi:10.1103/PhysRevA.51.1015.

[15] L. G. Valiant. Quantum computers that can be simulated classically in polynomial time. *Proceedings of the 33rd Annual ACM Symposium on Theory of Computing* 2001; pp. 114–123. doi:10.1145/380752.380785.

[16] B. M. Terhal, D. P. DiVincenzo. Classical simulation of noninteracting-fermion quantum circuits. *Physical Review A* 2002; **65**(3):032325. arXiv:quant-ph/0108010. doi:10.1103/PhysRevA.65.032325.

[17] D. E. Knuth. The Art of Computer Programming. 3rd Edition. Vol. 1. Addision-Wesley, Reading, Massachusetts, 1997.

[18] R. Garnier, J. Taylor. Discrete Mathematics: Proofs, Structures and Applications. 3rd Edition. CRC Press, Boca Raton, 2009. doi:10.1201/9781439812815.

[19] J. H. Conway. Regular Algebra and Finite Machines. Chapman and Hall, London, 1971.

[20] M. Sipser. Introduction to the Theory of Computation. 3rd Edition. Cengage, Boston, 2012.

[21] F. Wilczek. Majorana returns. *Nature Physics* 2009; **5**(9):614–618. doi:10.1038/nphys1380.

[22] R. Jozsa, A. Miyake. Matchgates and classical simulation of quantum circuits. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences* 2008; **464**(2100):3089–3106. arXiv:0804.4050. doi:10.1098/rspa.2008.0189.

[23] R. Jozsa, B. Kraus, A. Miyake, J. Watrous. Matchgate and space-bounded quantum computations are equivalent. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences* 2010; **466**(2115):809–830. arXiv:0908.1467. doi:10.1098/rspa.2009.0433.

[24] D. J. Brod. Efficient classical simulation of matchgate circuits with generalized inputs and measurements. *Physical Review A* 2016; **93**(6):062332. arXiv:1602.03539. doi:10.1103/PhysRevA.93.062332.

[25] A. Y. Vlasov. Quantum circuits and Spin(3n) groups. *Quantum Information and Computation* 2015; **15**(3-4):235–259. arXiv:1311.1666. doi:10.26421/qic15.3-4-3.

[26] S. Lorenzo, T. J. G. Apollaro, S. Paganelli, G. M. Palma, F. Plastina. Transfer of arbitrary two-qubit states via a spin chain. *Physical Review A* 2015; **91**(4):042321. arXiv:1502.02458. doi:10.1103/PhysRevA.91.042321.

[27] J. T. Seeley, M. J. Richard, P. J. Love. The Bravyi–Kitaev transformation for quantum computation of electronic structure. *Journal of Chemical Physics* 2012; **137**(22):224109. arXiv:1208.5986. doi:10.1063/1.4768229.

[28] A. Tranter, S. Sofia, J. Seeley, M. Kaicher, J. McClean, R. Babbush, P. V. Coveney, F. Mintert, F. Wilhelm, P. J. Love. The Bravyi–Kitaev transformation: Properties and applications. *International Journal of Quantum Chemistry* 2015; **115**(19):1431–1441. doi:10.1002/qua.24969.