

Effective Simulation of State Distribution in Qubit Chains

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Abstract

This work recollects a non-universal set of quantum gates described by higher-dimensional Spin groups. They are also directly related with matchgates in theory of quantum computations and complexity. Various processes of quantum state distribution along a chain such as perfect state transfer and different types of quantum walks can be effectively modeled on classical computer using such approach.

1 Introduction

The non-universal sets of quantum gates discussed in this work are known in the wide variety of contexts from matchgates in theory of complexity to Majorana modes in the solid body physics [1, 2, 3, 4, 5, 6, 7, 8, 9, 10], but they were often considered rather as *possible obstacles* for construction of general purpose quantum computers.

For example, such a non-universal set was described by the author as some auxiliary effect of construction of the universal set of quantum gates [6] inspired by an earlier work with an application of spinors and Clifford algebra formalism [11]. In the works about Majorana modes [4, 5] similar non-universal quantum gates are described by Hamiltonians with second-order terms and it was noted about “physical implementation” that an additional “four-particle interaction” necessary for universal quantum computation “will be particularly difficult to realize.”

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However, the model under consideration can be treated in the *more constructive way*. The matchgates was initially introduced in the theory of complexity as a special set of quantum gates simulated classically in polynomial time [1] and equivalence of the nearest-neighbor (n.n.) unitary matchgates with the non-universal set discussed above was proved soon [2, 3].

Here the term “matchgates” is often used for historical reasons and for the consistency with works of other authors. The spinor representation [6] reintroduced in Sect. 4 can be more convenient for the purposes of presented work. A similar approach with 2^n -components spinors was also briefly mentioned in [12] in relation with Majorana modes and ‘topological quantum computations’ [4, 13].

The spinorial approach also let us avoid necessity to digress into explanation of some special cases irrelevant to presented work. For example, without n.n. condition the matchgates can perform universal quantum computation [2, 7] that may not be effectively simulated classically. Originally suggested in [1] nearest-neighbor matchgates also could include non-physical (non-unitary and non-invertible) gates that should be discussed elsewhere [9].

The considered models are relevant not only to effective *classical* simulations of matchgate circuits. An equivalence of match-circuits of width n and an universal *quantum* computer with “exponentially compressed” number of qubits $O(\log(n))$ was shown in [8].

Thus, many problems in the theory of quantum information let us also consider the possibility of effective implementation of some restricted set of quantum circuits with such gates *as some benefit* for simulation, comparison of classical and quantum computational complexity and other tasks.

An application of this particular class of effectively simulated quantum circuits as a model of state distribution along a chain of qubits is considered in this work. The different types of quantum chains are introduced in Sect. 2 together with examples of processes appropriate for effective modeling such as perfect state transfer and different types of continuous and discrete quantum walks.

The *local representation* of a single link is discussed in Sect. 3 for establishing relation between a qubit chain and a simpler *scalar* model with dimension of Hilbert space is equal to number of nodes. It is used further in Sect. 4 for a *spinorial* description of Hamiltonians and the quantum evolution of the entire chain. The applications to the state distribution are summarized and extended for the multi-particle case in Sect. 5.

2 Quantum chains

2.1 Chain types

A *chain* is defined by a set of nodes $k = 1, \dots, n$ together with the pairs for representation of links. The usual (linear) chain is defined by the links $(k, k+1)$, $k = 1, \dots, n-1$. A *ring*, *i.e.*, *circular chain* has an additional link $(n, 1)$.

The *qubit chain* is formally equivalent to a quantum computational network with n qubits and quantum gates acting either on the single qubit or on the nearest neighbors $(k, k+1)$, $k = 1, \dots, n-1$. Additional two-gates for the pair of qubits $(1, n)$ at the ends of the chain produces the *qubit ring*. For the systems with n qubits the dimension of a space of states $\mathcal{H} = \mathcal{H}_2 \otimes \dots \otimes \mathcal{H}_2$ is 2^n and methods of effective classical simulation should not work *directly* with this exponentially large space.

A couple of related models is also considered together with the chain of qubits in this work. The *scalar quantum chains and rings* with n nodes are described by n -dimensional space \mathcal{H}_n . The *coined (discrete) quantum walk* [14, 15, 16, 17, 18] is equipped with two-dimensional *control space* and the space of states for this model is $\mathcal{H}_2 \otimes \mathcal{H}_n \simeq \mathcal{H}_{2n}$.

2.2 Coined quantum walk on scalar chain

The simple models of coined quantum walks on a line or a circle have the straightforward implementation using the scalar quantum chain with the doubled number of nodes. Let us start with the infinite quantum chain $|k\rangle$ with arbitrary integer indexes of nodes $k \in \mathbb{Z}$ to postpone the consideration of boundary conditions. Two operators for exchanging pairs of nodes may be introduced

$$\hat{S}_1: |2k\rangle \leftrightarrow |2k+1\rangle, \quad \hat{S}_2: |2k+1\rangle \leftrightarrow |2k+2\rangle. \quad (1)$$

Let us consider the composition \hat{S}_{12} of the operators \hat{S}_1 and \hat{S}_2

$$\hat{S}_{12}: \begin{cases} |2k\rangle \rightarrow |2k+1\rangle \rightarrow |2k+2\rangle \\ |2k+1\rangle \rightarrow |2k\rangle \rightarrow |2k-1\rangle \end{cases} \quad (2)$$

The action of Eq. 2 can be considered as two independent shifts with the double step in the opposite directions for odd and even indexes. For the

comparison with the model of a coined quantum walk, the nodes can be reordered into two infinite chains using the notation $|c\rangle|k\rangle$ for $|2k+c\rangle$ where $k \in \mathbb{Z}$, $c = 0, 1$. In such a case the operation \hat{S}_{12} Eq. 2 corresponds to the transformation

$$|0, k\rangle \rightarrow |0, k+1\rangle, \quad |1, k\rangle \rightarrow |1, k-1\rangle. \quad (3)$$

and may be rewritten as

$$\hat{S}_{12} = |0\rangle\langle 0| \otimes \hat{R} + |1\rangle\langle 1| \otimes \hat{L}, \quad (4)$$

where \hat{R} and \hat{L} denote right and left shifts $|k\rangle \rightarrow |k \pm 1\rangle$ respectively.

The operators such as Eq. 4 is an example of *conditional quantum dynamics* [19] with a *control qubit* $|c\rangle$ and a chain as a *target subsystem*. The same model is widely used for the *coined quantum walk* [14, 15, 16] with *coin flips* operators \hat{C} acting on the control qubit [15, 16]

$$\hat{W} = \hat{S}_{12}(\hat{C} \otimes \hat{I}), \quad (5)$$

where \hat{I} is the identity (unit) operator on the chain. In the initial notation with the single chain (before decomposition on control and target subsystems) the coin operator \hat{C} acts on the same pairs of nodes as \hat{S}_1 . So the coined quantum walk may be described by an analogue of the two-step method Eq. 1 with $\hat{S}'_1 = \hat{S}_1\hat{C}$ also known due to staggered and Szegedy quantum walks [20, 21, 22, 23].

A case of a circular quantum chain with $2n$ nodes is analogous with the infinite model considered above. The swap transformations S_1 and S_2 are defined similarly with Eq. 1 using addition modulo $2n$. The relation between such a chain and a coined quantum walk on a circle with n nodes again corresponds to the reordering $|c\rangle|k\rangle$ for $|2k+c\rangle$ where $k = 0, \dots, n-1$, $c = 0, 1$ and arithmetic modulo n is used for the second index in Eq. 3. The expression Eq. 4 should be rewritten in such a case using $n \times n$ the matrix \hat{U}_n of the cyclic shift

$$\hat{S}_{12} = |0\rangle\langle 0| \otimes \hat{U}_n + |1\rangle\langle 1| \otimes \hat{U}_n^\dagger. \quad (4')$$

The boundary conditions for a linear chain with $2n$ nodes is a bit more difficult. Here the operations \hat{S}_1 and \hat{S}_2 in Eq. 1 should be modified for the ends of the chain. The bounded analogues should not affect nodes outside of

the range $1, \dots, 2n - 1$. After the transition to the coined quantum walk on a line with n nodes such an approach produces specific reflection effects on the boundaries.

Very similar models were used for graphs with more general structure for approaches with staggered and Szegedy quantum walks [20, 21, 22, 23], but it is not well suited to the consideration of an effective simulation model discussed further.

2.3 Continuous quantum walk on chains

Let us consider an alternative model of the *continuous quantum walk* [17, 18, 24] also applicable to the consideration of the *perfect state transport* [25, 26, 27, 28]. The methods are relevant both for scalar and qubit chains.

The scalar chain is encoded by qubits adapting of the standard approach from the theory of spin waves [29, 32, 33]. Inside of the whole 2^n -dimensional Hilbert space of system with n qubits a state of the chain can be mapped into n -dimensional subspace spanned by states with a single unit in the computational basis

$$|k\rangle \equiv \underbrace{|0 \dots 0 1 0 \dots 0\rangle}_{k-1}, \quad k = 1, \dots, n. \quad (6)$$

In such a model the element \hat{H}_{jk} of Hamiltonians is nonzero only for the linked nodes j and k . A simple example is an adjacency matrix of graphs with unit elements for the edges. For linear and circular chains Hamiltonians defined by an adjacency matrix are quite simple and may be presented respectively as \hat{H}^1 and \hat{H}^c with the only nonzero elements

$$\begin{aligned} \hat{H}_{k,k-1}^1 &= \hat{H}_{k-1,k}^1 = 1, & k &= 1, \dots, n-1, \\ \hat{H}_{k \bmod n, k-1}^c &= \hat{H}_{k-1, k \bmod n}^c = 1, & k &= 1, \dots, n. \end{aligned}$$

In the model discussed earlier an evolution of a chain on each discrete step was represented by the unitary operators $|\psi\rangle \rightarrow \hat{U}|\psi\rangle$. A similar approach for models with given Hamiltonian may be developed by choice of the fixed time step τ . The evolution of a chain for each step is described by the operator

$$\hat{U}(\tau) = \exp(-i\hat{H}\tau) \quad (7)$$

and in a general case only for $\tau \rightarrow 0$ the structure of the links represented by the Hamiltonian is simply related with the evolution after the single step due to $\hat{U}(\tau) \approx \hat{I} - i\hat{H}\tau$.

Evolution due to the Hamiltonian constructed from the adjacency matrix for finite τ corresponds to a state propagation along connected paths in the graph described by the links. For the qubit chain such a model may produce too complex gates acting on arbitrary big number of qubits.

The problem can be partially resolved by using short chains with two and three qubits as the building blocks [26]. On the other hand, some Hamiltonians with the specific values instead of units in the adjacency matrix may produce the transport of a localized state for particular values of τ , *i.e.*, after some period of time such an evolution is formally equivalent to the swap gate applied to the ends of the chain [26, 27]. For a scalar quantum chain with n nodes a neat example is an evolution described by the Hamiltonian with only nonzero elements for adjacent nodes

$$\hat{H}_{k,k-1} = \hat{H}_{k-1,k} = \frac{1}{2}\sqrt{k(n-k)}, \quad k = 1, \dots, n-1. \quad (8)$$

The model is quite illustrative due to the possibility to map nodes into states of a quantum particle with the spin $s = (n-1)/2$. A node with an index $k = 0, \dots, n-1$ would correspond to the spin projection $s_z = (-s/2 + k)\hbar$ on z axis of such a formal quantum system. The *natural system of units* with $\hbar = 1$ is used further for simplicity.

Such a Hamiltonian may be simply interpreted as a rotation of a particle with the spin $s = (n-1)/2$ along x axis [29] and so the state *spin up* with the projection $s_z = +s/2$ evolves into the state *spin down* $s_z = -s/2$. The formal spin model is convenient for the consideration of the quantum chain not only because elements of the Hamiltonian correspond to the next-neighbor structure, but also due to the quite straightforward expression for the evolution Eq. 7.

A spin-half particle is the simple example corresponding to a chain with two nodes or the qubit $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$. The change of a state due to rotation corresponds to some unitary 2×2 matrix $|\psi'\rangle = \hat{U}|\psi\rangle$. Let us consider n -dimensional linear space of polynomials of order $n-1$ with two variables α, β with the basis

$$p_k(\alpha, \beta) = \sqrt{\frac{(n-1)!}{k!(n-k-1)!}}\alpha^k\beta^{n-k-1} = \sqrt{C_{n-1}^k}\alpha^k\beta^{n-k-1}, \quad (9)$$

where $k = 0, \dots, n-1$. The transformation of such polynomials due to application of an unitary 2×2 matrix U to the coefficients (α, β) of a qubit mentioned earlier describes rotation of the formal system with the spin s

[29, 36]. The coefficients $\sqrt{C_{n-1}^k}$ in Eq. 9 ensure unitarity of the $n \times n$ transformation matrix.

The initial state $|0\rangle$ with $\alpha = 1, \beta = 0$ produces only one nonzero polynomial p_0 . The quantum *NOT* gate transforms $|0\rangle \rightarrow |1\rangle$ with $\alpha = 0, \beta = 1$ and only nonzero polynomial p_{n-1} . If states of the formal spin system are mapped into a chain with $n = 2s+1$ nodes such a transformation corresponds to the exchange of values between two end nodes $|1\rangle$ and $|n\rangle$. On the other hand, the gate may be implemented by continuous spin rotation around x axis using the Hamiltonian Eq. 8.

The same gate may be implemented using rotation around y axis. In such a case all nonzero elements of the Hamiltonian are pure imaginary. Models of the state transport often utilize real Hamiltonian such as Eq. 8 and a more general case with complex coefficients is adapted for the *chiral quantum walks* [30, 31]. Here is useful to compare the Hamiltonian $\hat{H} = \hat{H}^x$ Eq. 8 with \hat{H}^y and \hat{H}^z representing rotations around y and z axis. The nonzero elements may be expressed by equations

$$\begin{aligned}\hat{H}_{k,k-1}^x &= \hat{H}_{k-1,k}^x = i\hat{H}_{k,k-1}^y = -i\hat{H}_{k-1,k}^y = \frac{1}{2}\sqrt{k(n-k)} \\ \hat{H}_{k,k}^z &= k - \frac{1}{2}(n-1).\end{aligned}\tag{10}$$

An arbitrary rotation is represented by the linear combination of the three Hamiltonians $\hat{H}_\lambda = \lambda_x \hat{H}^x + \lambda_y \hat{H}^y + \lambda_z \hat{H}^z$, but the perfect transfer may be implemented only for rotation around an axis perpendicular to z for $\lambda_z = 0$.

3 Comparison of scalar and qubit chains

Let us consider the relation between scalar and qubit chains. The quantum circuit model is convenient for the initial consideration of the *single link with two nodes*. The space of states for two qubits is four-dimensional and transitions should not change the number of units in the computational basis. The nontrivial evolution is only between $|01\rangle$ and $|10\rangle$, but other two states may only change phases.

The matrix of the transformation can be represented in general as

$$M = \begin{pmatrix} e^{i\nu} & 0 & 0 & 0 \\ 0 & \mu_{11} & \mu_{12} & 0 \\ 0 & \mu_{21} & \mu_{22} & 0 \\ 0 & 0 & 0 & e^{i\nu'} \end{pmatrix}\tag{11}$$

Let us recall that the matchgate [1, 2, 3, 7, 8] is a quantum two-gate with 4×4 matrix composed from elements of two matrices $A, B \in \text{SU}(2)$

$$e^{i\theta} M(A, B) = \begin{pmatrix} A_{11} & 0 & 0 & A_{12} \\ 0 & B_{11} & B_{12} & 0 \\ 0 & B_{21} & B_{22} & 0 \\ A_{21} & 0 & 0 & A_{22} \end{pmatrix} \quad (12)$$

The matrix of the transformation Eq. 11 corresponds to Eq. 12 for $\theta = -(\nu + \nu')/2$ and

$$A = \begin{pmatrix} e^{i(\nu-\nu')/2} & 0 \\ 0 & e^{i(\nu'+\nu)/2} \end{pmatrix}, \quad (13a)$$

$$B = e^{-i\theta} \begin{pmatrix} \mu_{11} & \mu_{12} \\ \mu_{21} & \mu_{22} \end{pmatrix}. \quad (13b)$$

An element of $\text{SU}(2)$ group can be expressed as

$$U = \begin{pmatrix} \alpha & \beta \\ -\bar{\beta} & \bar{\alpha} \end{pmatrix}, \quad |\alpha|^2 + |\beta|^2 = 1 \quad (14)$$

and an element of $\text{U}(2)$ may include a multiplier $e^{-i\theta}$.

The additional requirement about two $\text{SU}(2)$ matrices with the unit determinant or $\det(A) = \det(B) = e^{-i\theta}$ for the more general case with $\text{U}(2)$ is not related with discussed earlier properties of links between nodes in the chain. Such a subtlety is essential further for consideration of effective simulations.

For example, an exchange or the *SWAP* gate

$$\hat{P} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (15)$$

does not satisfy the requirement about equality of determinants. The permission to include *SWAP* would expand matchgates from nearest neighbors to arbitrary pairs of qubits, but the extended set of quantum gates is universal with lack of possibility for the effective classical simulations [7, 8].

An alternative is some “signed” *SWAP* such as

$$\hat{P}_- = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad (16)$$

corresponding to the general case of Eq. 12 with the phase $\theta = \pi$. Such a matchgate Eq. 16 does not change a sign for the states $|k\rangle$ Eq. 6 with a single unit in the computational basis.

The model with Hamiltonians clarifies description of some properties [2, 7]. For two-dimensional (sub)space of states the exponential expression Eq. 7 generates elements of $U(2)$ for decomposition of Hamiltonians with Pauli matrices

$$\hat{H}_2(\boldsymbol{\lambda}) = \lambda_0 \hat{I}_2 + \lambda_1 \hat{\sigma}^x + \lambda_2 \hat{\sigma}^y + \lambda_3 \hat{\sigma}^z \quad (17)$$

for real $\lambda_k \in \mathbb{R}$. Here \hat{I}_2 is 2×2 identity matrix and the requirement about the unit determinant for $SU(2)$ corresponds to $\lambda_0 = 0$.

Hamiltonians in Eq. 7 for generating of matrices, satisfying both Eq. 11 and Eq. 13 can be expressed as

$$\hat{H}_4(\theta, \boldsymbol{\lambda}) = \lambda_0 \hat{I}_4 + \lambda_1 \hat{\Sigma} + \lambda_2 \hat{\Lambda} + \lambda_3 \hat{\Delta} + \theta \hat{\Delta}', \quad (18)$$

where \hat{I}_4 is 4×4 identity matrix and the terms in Eq. 18 can be represented with Pauli matrices

$$\hat{\Sigma} = \frac{\hat{\sigma}^x \otimes \hat{\sigma}^x + \hat{\sigma}^y \otimes \hat{\sigma}^y}{2} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (19a)$$

$$\hat{\Lambda} = \frac{\hat{\sigma}^y \otimes \hat{\sigma}^x - \hat{\sigma}^x \otimes \hat{\sigma}^y}{2} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (19b)$$

$$\hat{\Delta} = \frac{\hat{\sigma}^z \otimes \hat{I}_2 - \hat{I}_2 \otimes \hat{\sigma}^z}{2} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (19c)$$

$$\hat{\Delta}' = \frac{\hat{\sigma}^z \otimes \hat{I}_2 + \hat{I}_2 \otimes \hat{\sigma}^z}{2} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \quad (19d)$$

The Hamiltonian for a more general matrix from Eq. 11 without the requirement about the unit determinant may also include the term

$$\hat{\Theta} = \frac{\hat{I}_4 - \hat{\sigma}^z \otimes \hat{\sigma}^z}{2} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (20)$$

Finally, the Hamiltonian for the most general matchgate Eq. 12 would require two additional terms

$$\hat{\Sigma}' = \frac{\hat{\sigma}^x \otimes \hat{\sigma}^x - \hat{\sigma}^y \otimes \hat{\sigma}^y}{2} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad (21a)$$

$$\hat{\Lambda}' = \frac{\hat{\sigma}^y \otimes \hat{\sigma}^x + \hat{\sigma}^x \otimes \hat{\sigma}^y}{2} = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}, \quad (21b)$$

For a single link with two qubits relations between Hamiltonians and quantum gates can be simplified in such representations due to analogies with the single qubit case using correspondence between Pauli matrices ($\hat{\sigma}^x, \hat{\sigma}^y, \hat{\sigma}^z$) and triples $(\hat{\Sigma}, \hat{\Lambda}, \hat{\Delta})$ or $(\hat{\Sigma}', \hat{\Lambda}', \hat{\Delta}')$.

The notation such as Eq. 19 used for the triples does not look uniform with respect to all three Pauli matrices, but it is intended to indicate some properties of the whole chain. Indeed, let us rewrite the *spin exchange* operator Eq. 15

$$\hat{P} = \frac{\hat{I}_4 + \hat{\sigma}^x \otimes \hat{\sigma}^x + \hat{\sigma}^y \otimes \hat{\sigma}^y + \hat{\sigma}^z \otimes \hat{\sigma}^z}{2}. \quad (15')$$

The expression Eq. 15' is isotropic, *i.e.*, invariant with respect to a 3D rotation \mathbf{R}

$$\hat{\sigma}^\alpha \mapsto \sum_{\alpha, \beta} \mathbf{R}_{\alpha\beta} \hat{\sigma}^\beta, \quad \alpha, \beta = x, y, z. \quad (22)$$

Four terms Eq. 19 are anisotropic due to the preferred axis z in the computational basis, but a reduced symmetry still presents with respect to 2D rotations in xy plane around z .

For $\hat{\Sigma}$ and $\hat{\Lambda}$ in Eqs. 19a, 19b such an invariance may be formally derived from the conservation of 2D length and area respectively. Two other terms Eq. 21 do not have even such a reduced symmetry.

A particular case of $\pi/2$ rotation around z -axis is essential for the further applications and denoted here as

$$\mathcal{J}: (\hat{\sigma}_k^x, \hat{\sigma}_k^y, \hat{\sigma}_k^z) \mapsto (-\hat{\sigma}_k^y, \hat{\sigma}_k^x, \hat{\sigma}_k^z). \quad (23)$$

Such a transformation does not affect Eq. 19, but it changes signs of terms in Eq. 21.

For the representation with Hamiltonians such as Eq. 18 an evolution of the whole chain is described by the exponent Eq. 7 with the sum or the linear combination of the terms for all existing links. The term $\hat{\Sigma}$ in Eq. 19a corresponds to the Heisenberg XY spin chain and quite common in the models of the perfect state transport [26, 27] and quantum computing [33]. The pure imaginary term Eq. 19b can be treated as a “chiral” [30, 31] or “spiral” [34] and may appear due to the Dzyaloshinskii-Moriya interaction [35]. A model with the local magnetic field has additional terms $\hat{\sigma}_z$ acting on single qubits [26, 27, 33] related with Eqs. 19c, 19d due to the obvious grouping $\hat{\Delta} \pm \hat{\Delta}'$. Finally, the Hamiltonian for a chain with terms Eq. 19 may be written as

$$\begin{aligned} \hat{H} &= \sum_{k=1}^{n-1} \frac{\alpha_k}{2} (\hat{\sigma}_k^x \hat{\sigma}_{k+1}^x + \hat{\sigma}_k^y \hat{\sigma}_{k+1}^y) \\ &+ \sum_{k=1}^{n-1} \frac{\beta_k}{2} (\hat{\sigma}_k^y \hat{\sigma}_{k+1}^x - \hat{\sigma}_k^x \hat{\sigma}_{k+1}^y) + \sum_{k=1}^n \delta_k \hat{\sigma}_k^z. \end{aligned} \quad (24)$$

The alternative model with gates discussed earlier has some subtlety, when a result of a step may not be expressed naturally because of noncommuting operators. In such a case

$$\exp(\hat{A} + \hat{B}) \neq \exp(\hat{A}) \exp(\hat{B})$$

and a sum of Hamiltonians acting on overlapped pairs of qubits after the exponentiation Eq. 7 in general produces n -qubit operator without obvious relation with gates for initial pairs. Decomposition of such operator on two-qubit gates may be a difficult task.

A formal resolution of the problem is the decomposition on different steps with only commuting operators in each one. The partition of a graph on

links without common nodes is an easy way to ensure commutativity. The alternative expression with two operators Eq. 5 for coined quantum walk is a simple example. The approach with partitions is widely used for discrete time quantum walks [20, 21, 22].

The application of a similar model for qubit chains may be considered as a special case of quantum cellular automata with the Margolus partitioning scheme [37].

4 Spinorial evolution of qubit chain

4.1 Clifford algebras and Spin groups

The matchgates Eq. 12 were already adapted above Eq. 13 together with the matrix Eq. 11 used for the description of transition between scalar and qubit chains. The nearest neighbor matchgates were exploited for the description of quantum circuits effectively modeled on a classical computer [1, 2, 3, 7, 8, 9, 10]. The term “matchgates” is used here for compatibility with other works and some historical reasons, but further methods rely on rather standard theory of Clifford algebras and Spin groups [39, 40].

The Hamiltonians for nearest neighbor matchgates can be expressed with $2n$ anticommuting generators of the Clifford algebra [2, 7] also known due to the Jordan-Wigner transformation [38]. The relation corresponds to the standard representation of Spin groups [6, 40].

The similar approach also appears earlier due to natural analysis of universality using Hamiltonians of quantum gates [41], because a non-universal set of gates was directly related with Clifford algebras and Spin groups of multidimensional Euclidean spaces [4, 5, 6, 12].

The Clifford algebra $\mathcal{Cl}(m)$ of m -dimensional Euclidean space is defined by m generators \mathbf{e}_k with relations [40]

$$\mathbf{e}_j \mathbf{e}_k + \mathbf{e}_k \mathbf{e}_j = -2\delta_{jk} \mathbf{1}, \quad k, j = 1, \dots, m \quad (25)$$

The 2^m -dimensional algebra $\mathcal{Cl}(m)$ is spanned by different products of \mathbf{e}_k . The linear span of generators \mathbf{e}_k maps initial Euclidean space into m -dimensional subspace \mathcal{V} of $\mathcal{Cl}(m)$ and due to Eq. 25 the Euclidean norm of $\mathbf{v} \in \mathcal{V}$ satisfies $|\mathbf{v}|^2 = -\mathbf{v}^2$.

The Spin(m) group is defined by all possible products with *even* number of elements from \mathcal{V} with unit norm. The products of *arbitrary* number of such elements define group Pin(m) [40].

The important property of Spin group is relation with group of rotations $\text{SO}(m)$, because for any $\mathbf{R} \in \text{SO}(m)$ the rotation

$$\mathbf{v}' = \mathbf{R}\mathbf{v}, \quad \mathbf{v}'_k = \sum_{j=1}^m \mathbf{R}_{kj} \mathbf{v}_j \quad (26)$$

may be rewritten as the *adjoint action*

$$\mathbf{v}' = \mathcal{S}_\mathbf{R} \mathbf{v} \mathcal{S}_\mathbf{R}^{-1} \equiv \text{Ad}_{\mathcal{S}_\mathbf{R}}(\mathbf{v}), \quad \mathcal{S}_\mathbf{R} \in \text{Spin}(m). \quad (27)$$

Here two elements $\pm \mathcal{S}_\mathbf{R}$ correspond to the same rotation \mathbf{R} and Eq. 27 defines 2-fold homomorphism, *i.e.*, a map respecting the composition of transformations. For effective simulations further is essential a reciprocal opportunity to use rotations for the work with quantum circuits represented by the Spin group. For the generators from Eq. 26 and Eq. 27 follows

$$\mathcal{S}_\mathbf{R} \mathbf{e}_k \mathcal{S}_\mathbf{R}^{-1} = \sum_{j=1}^m \mathbf{R}_{kj} \mathbf{e}_j. \quad (28)$$

In even dimension $m = 2n$ the generators can be expressed with the Jordan-Wigner method [38, 40]

$$\mathbf{e}_k = i \underbrace{\hat{\sigma}^z \otimes \cdots \otimes \hat{\sigma}^z}_{k-1} \otimes \hat{\sigma}^x \otimes \underbrace{\hat{I}_2 \otimes \cdots \otimes \hat{I}_2}_{n-k}, \quad (29a)$$

$$\mathbf{e}_{k+n} = i \underbrace{\hat{\sigma}^z \otimes \cdots \otimes \hat{\sigma}^z}_{k-1} \otimes \hat{\sigma}^y \otimes \underbrace{\hat{I}_2 \otimes \cdots \otimes \hat{I}_2}_{n-k}, \quad (29b)$$

where $k = 1, \dots, n$. An alternative short notation is useful further

$$\mathbf{e}_k = i \hat{\sigma}_1^z \cdots \hat{\sigma}_{k-1}^z \hat{\sigma}_k^x, \quad \mathbf{e}_{k+n} = i \hat{\sigma}_1^z \cdots \hat{\sigma}_{k-1}^z \hat{\sigma}_k^y. \quad (30)$$

The expressions Eq. 19 for two neighboring qubits may be rewritten with Eq. 30

$$\hat{\Sigma}_{k,k+1} = \frac{\mathbf{e}_k \mathbf{e}_{k+n+1} + \mathbf{e}_{k+1} \mathbf{e}_{k+n}}{2i}, \quad (31a)$$

$$\hat{\Lambda}_{k,k+1} = \frac{\mathbf{e}_k \mathbf{e}_{k+1} + \mathbf{e}_{k+n} \mathbf{e}_{k+n+1}}{2i}, \quad (31b)$$

$$\hat{\Delta}_{k,k+1} = \frac{\mathbf{e}_k \mathbf{e}_{k+n} - \mathbf{e}_{k+1} \mathbf{e}_{k+n+1}}{2i}, \quad (31c)$$

$$\hat{\Delta}'_{k,k+1} = \frac{\mathbf{e}_k \mathbf{e}_{k+n} + \mathbf{e}_{k+1} \mathbf{e}_{k+n+1}}{2i}. \quad (31d)$$

Supplementary Hamiltonians Eq. 21 needed for the representation of arbitrary matchgates can be rewritten as

$$\hat{\Sigma}'_{k,k+1} = \frac{\mathbf{e}_k \mathbf{e}_{k+n+1} - \mathbf{e}_{k+1} \mathbf{e}_{k+n}}{2i}, \quad (32a)$$

$$\hat{\Lambda}'_{k,k+1} = \frac{\mathbf{e}_k \mathbf{e}_{k+1} - \mathbf{e}_{k+n} \mathbf{e}_{k+n+1}}{2i}, \quad (32b)$$

An analogue of $\hat{\Theta}$ Eq. 20 may not be expressed in a similar way, because it requires four Clifford generators

$$\hat{\Theta}_{k,k+1} = \frac{\mathbf{1} + \mathbf{e}_k \mathbf{e}_{k+n} \mathbf{e}_{k+1} \mathbf{e}_{k+n+1}}{2}. \quad (33)$$

The exchange operator \hat{P} Eq. 15' also requires four Clifford generators, but a “signed” version \hat{P}_- might be expressed using Eq. 31.

It may be convenient to consider a more general definition for Eq. 31

$$\hat{\Sigma}_{k,j} = \frac{\mathbf{e}_k \mathbf{e}_{j+n} + \mathbf{e}_j \mathbf{e}_{k+n}}{2i}, \quad (34a)$$

$$\hat{\Lambda}_{k,j} = \frac{\mathbf{e}_k \mathbf{e}_j + \mathbf{e}_{k+n} \mathbf{e}_{j+n}}{2i}. \quad (34b)$$

Both $\hat{\Delta}_{k,k+1}$ and $\hat{\Delta}'_{k,k+1}$ may be expressed in terms of Eq. 34a due to the identity

$$\hat{\sigma}_k^z = -i \mathbf{e}_k \mathbf{e}_{k+n} = \hat{\Sigma}_{k,k}. \quad (35)$$

4.2 Admissible evolution of qubit chain

The evolution of a qubit chain considered above preserves the subspace spanned by states $|k\rangle$ Eq. 6 with a single unit in the computational basis. Linear combinations of Hamiltonians Eq. 19 for nearest neighbor qubits generate transformations respecting such a subspace and compositions of corresponding quantum gates Eq. 11 also have the necessary property. For the certainty the term *admissible* is used further for such an evolution, relevant quantum gates, Hamiltonians and elements of Spin group.

Let us use expressions Eq. 31 with elements of the Clifford algebra. A replacement of n pairs

$$\mathbf{e}_k \mapsto -\mathbf{e}_{k+n}, \quad \mathbf{e}_{k+n} \mapsto \mathbf{e}_k, \quad k = 1, \dots, n \quad (36)$$

does not change operators Eq. 31, but it alternates signs in Eq. 32. Such properties may be simply checked using the analogue transformation with Pauli matrices introduced earlier Eq. 23.

The substitution Eq. 36 can be treated as $2n \times 2n$ matrix

$$\mathbf{J} = \begin{pmatrix} \mathbf{0}_n & \mathbf{1}_n \\ -\mathbf{1}_n & \mathbf{0}_n \end{pmatrix}, \quad (37)$$

where $\mathbf{0}_n, \mathbf{1}_n$ denote $n \times n$ zero and unit matrices, respectively. Because \mathbf{J} is orthogonal matrix, Eq. 36 also may be rewritten as Eq. 27 for the adjoint action $\text{Ad}_{\mathcal{J}}$ with the element \mathcal{J} of the Spin group expressed as the composition of n elementary terms derived from Eq. 36

$$\mathcal{J} = \frac{1}{\sqrt{2^n}} \prod_{k=1}^n (1 - \mathbf{e}_k \mathbf{e}_{k+n}) = \frac{1}{\sqrt{2^n}} \prod_{k=1}^n (\hat{I} + i \hat{\sigma}_k^z). \quad (38)$$

Admissible Hamiltonians \hat{H}_a for the evolution of a chain are expressed as linear combinations of elements Eq. 31. Such Hamiltonians satisfy $\hat{H}_a = \text{Ad}_{\mathcal{J}}(\hat{H}_a) = \mathcal{J} \hat{H}_a \mathcal{J}^{-1}$, *i.e.*, they commute with the element \mathcal{J}

$$\hat{H}_a \mathcal{J} = \mathcal{J} \hat{H}_a. \quad (39)$$

Due to Eq. 7 the evolution of a quantum chain generated by such Hamiltonians also commutes with \mathcal{J} and the same is true for the particular case with nearest neighbor quantum gates such as Eq. 11 and for any circuit composed from them. Operators \hat{U}_a describing admissible evolution of a qubit chain due to such quantum gates and circuits also commute with \mathcal{J}

$$\hat{U}_a \mathcal{J} = \mathcal{J} \hat{U}_a. \quad (40)$$

Some properties of \mathcal{J} may be more convenient to explain using an operator

$$\hat{N}^z = \sum_{k=1}^n \frac{\hat{I} - \hat{\sigma}_k^z}{2} = \frac{n}{2} \hat{I} - \frac{1}{2} \sum_{k=1}^n \hat{\sigma}_k^z. \quad (41)$$

Any vector of the computational basis $|\Psi\rangle$ meets

$$\hat{N}^z |\Psi\rangle = N_{\Psi} |\Psi\rangle, \quad (42)$$

where N_{Ψ} is the number of units in a binary notation.

The relation between \hat{N}^z and \mathcal{J} may be expressed using Eq. 38 and Eq. 41

$$e^{i\frac{\pi}{4}n}e^{-i\frac{\pi}{2}\hat{N}^z} = \prod_{k=1}^n e^{i\frac{\pi}{4}\hat{\sigma}_k^z} = \prod_{k=1}^n \frac{\hat{I} + i\hat{\sigma}_k^z}{\sqrt{2}} = \mathcal{J} \quad (43)$$

Due to Eq. 42 $\hat{N}^z|\underline{k}\rangle = |\underline{k}\rangle$ for the basis of n -dimensional subspace Eq. 6 and the same is true for any elements of the subspace $|\underline{\psi}\rangle$ represented as a linear combination of the basic states

$$|\underline{\psi}\rangle = \sum_{k=1}^n \psi_k |\underline{k}\rangle, \quad \hat{N}^z|\underline{\psi}\rangle = |\underline{\psi}\rangle \quad (44)$$

The similar expressions Eq. 42 are valid for any subspace spanned by basic vectors with the fixed number of units in the computational basis. An operator \hat{U}_a respecting the numbers acts irreducibly on all such subspaces and commutes with both \hat{N}^z and \mathcal{J} due to Eq. 43.

4.3 Annihilation and creation operators

The admissible transformations described above correspond to some subgroup of the Spin group related with $2n \times 2n$ orthogonal matrices of rotations discussed earlier Eq. 27. The matrices are also *symplectic* due to commutation with \mathbf{J} Eq. 37 and they belong to *symplectic orthogonal group* $\text{OSp}(2n)$ [42].

A crucial property of $\text{OSp}(2n)$ is the isomorphism with the special unitary group $\text{SU}(n)$ [42]. Let us consider a correspondence between complex and real matrices written

$$\mathbf{M}_{\mathbb{C}} = \mathbf{M}_{\mathbb{R}} + i\mathbf{M}_{\mathbb{I}} \longleftrightarrow \mathbf{M}_{\mathbb{R}} = \begin{pmatrix} \mathbf{M}_{\mathbb{R}} & \mathbf{M}_{\mathbb{I}} \\ -\mathbf{M}_{\mathbb{I}} & \mathbf{M}_{\mathbb{R}} \end{pmatrix} \quad (45)$$

where $\mathbf{M}_{\mathbb{R}}$ and $i\mathbf{M}_{\mathbb{I}}$ are $n \times n$ matrices composed respectively from real and imaginary parts of elements $\mathbf{M}_{\mathbb{C}}$.

For the unitary matrix $\mathbf{U} = \mathbf{U}_{\mathbb{R}} + i\mathbf{U}_{\mathbb{I}} \in \text{SU}(n)$ the correspondence Eq. 45 produces the standard isomorphism [42] with $\mathbf{M}_{\mathbb{R}} = \mathbf{R}_{\mathbf{U}} \in \text{OSp}(2n)$

$$\mathbf{R}_{\mathbf{U}} = \begin{pmatrix} \mathbf{U}_{\mathbb{R}} & \mathbf{U}_{\mathbb{I}} \\ -\mathbf{U}_{\mathbb{I}} & \mathbf{U}_{\mathbb{R}} \end{pmatrix}. \quad (46)$$

For the exponential representation $\mathbf{U} = \exp(\mathbf{iH}\tau)$ with a Hermitian matrix \mathbf{H} the same procedure Eq. 45 should be applied to $\mathbf{M}_C = \mathbf{iH}$ producing a generator for an appropriate rotation.

The approach is also related with the Jordan-Wigner operators [36, 38, 40]

$$\hat{a}_k = \frac{\mathbf{e}_k + \mathbf{i}\mathbf{e}_{k+n}}{2\mathbf{i}}, \quad \hat{a}_k^\dagger = \frac{\mathbf{e}_k - \mathbf{i}\mathbf{e}_{k+n}}{2\mathbf{i}}. \quad (47)$$

The Eq. 47 meet the *canonical anticommutation relations* for fermionic annihilation and creation operators

$$\{\hat{a}_j, \hat{a}_k^\dagger\} = \delta_{jk}, \quad \{\hat{a}_j, \hat{a}_k\} = \{\hat{a}_j^\dagger, \hat{a}_k^\dagger\} = 0 \quad (48)$$

The approach to the effective simulation of quantum circuits based on these operators may be found in [2], but few points should be clarified here.

Transition from generators \mathbf{e}_k to operators Eq. 47 can be expressed formally by $2n \times 2n$ complex matrix

$$\Xi = \frac{1}{2} \begin{pmatrix} \mathbf{1}_n & \mathbf{i}\mathbf{1}_n \\ \mathbf{1}_n & -\mathbf{i}\mathbf{1}_n \end{pmatrix}. \quad (49)$$

For $\mathbf{R} \in \text{OSp}(2n)$ the matrix \mathbf{U}_Ξ produced by transformation Eq. 49 can be expressed directly using the unitary matrix \mathbf{U} introduced earlier Eq. 46

$$\mathbf{U}_\Xi = \Xi \mathbf{R}_U \Xi^{-1} = \begin{pmatrix} \mathbf{U}_\Re + \mathbf{i}\mathbf{U}_\Im & \mathbf{0}_n \\ \mathbf{0}_n & \mathbf{U}_\Re - \mathbf{i}\mathbf{U}_\Im \end{pmatrix} = \begin{pmatrix} \mathbf{U} & \mathbf{0}_n \\ \mathbf{0}_n & \bar{\mathbf{U}} \end{pmatrix} \quad (50)$$

In such representation the requirements about commutativity with \mathbf{J} become rather trivial due to diagonalization of the matrix

$$\mathbf{J}_\Xi = \Xi \mathbf{J} \Xi^{-1} = \mathbf{i} \begin{pmatrix} \mathbf{1}_n & \mathbf{0}_n \\ \mathbf{0}_n & -\mathbf{1}_n \end{pmatrix} \quad (51)$$

obviously commuting with any matrix Eq. 50.

Let us consider for the admissible chain evolution $\hat{\mathcal{U}} \equiv \mathcal{S}_R$ transformations of operators Eq. 47

$$\hat{a}'_k = \hat{\mathcal{U}} \hat{a}_k \hat{\mathcal{U}}^{-1}, \quad \hat{a}'_k{}^\dagger = \hat{\mathcal{U}} \hat{a}_k^\dagger \hat{\mathcal{U}}^{-1}. \quad (52)$$

Due to Eq. 26 and Eq. 28 it corresponds to formal complex transformations $\mathbf{a} = \Xi \mathbf{v}$, $\mathbf{a}' = \Xi \mathbf{v}'$ and

$$\mathbf{a}' = \Xi \mathbf{R} \Xi^{-1} \mathbf{a} = \mathbf{U}_\Xi \mathbf{a}. \quad (53)$$

Finally, the transformation Eq. 52 for the admissible evolution of the chain can be expressed as an analogue of Eq. 28

$$\hat{\mathcal{U}}\hat{a}_k\hat{\mathcal{U}}^\dagger = \sum_{j=1}^n \mathcal{U}_{kj}\hat{a}_j, \quad \hat{\mathcal{U}}\hat{a}_k^\dagger\hat{\mathcal{U}}^\dagger = \sum_{j=1}^n \bar{\mathcal{U}}_{kj}\hat{a}_j^\dagger. \quad (54)$$

similar with the *restricted case* of classical simulations considered in [2].

There is some analogy with linear optics also described by $\text{OSp}(2n)$ transformations of bosonic creation and annihilation operators discussed elsewhere [10, 43].

Quadratic expressions for Hamiltonians Eq. 34 also may be rewritten using fermionic operators

$$\hat{\Sigma}_{k,j} = \frac{\hat{a}_k\hat{a}_j^\dagger + \hat{a}_j\hat{a}_k^\dagger}{2}, \quad (55a)$$

$$\hat{\Lambda}_{k,j} = \frac{\hat{a}_k\hat{a}_j^\dagger - \hat{a}_j\hat{a}_k^\dagger}{2i}. \quad (55b)$$

5 Effective modeling of qubit chains

5.1 Single-particle simulation

The effective classical simulation of quantum circuits discussed here may use an expression Eq. 28 with earlier developed methods [7, 8] almost without modifications and decompositions Eq. 54 also provides an alternative approach similar with discussed in [2].

Let us consider a scheme appropriate for many cases discussed earlier [2, 7, 8, 10]. A quantum circuit is described by the unitary operator $\hat{\mathcal{U}}$ and composed from products of separate gates. It is applied to the initial state $|\psi_{\text{in}}\rangle$ with the final measurement of probabilities defined by some operator \hat{M}_{out}

$$p = \langle \psi_{\text{in}} | \hat{\mathcal{U}}^\dagger \hat{M}_{\text{out}} \hat{\mathcal{U}} | \psi_{\text{in}} \rangle = \text{Tr}(\hat{M}_{\text{out}} \hat{\mathcal{U}} \hat{\rho}_{\text{in}} \hat{\mathcal{U}}^\dagger), \quad (56)$$

where $\hat{\rho}_{\text{in}} = |\psi_{\text{in}}\rangle\langle\psi_{\text{in}}|$ is the density operator of the initial state. The expression with trace Tr can be also used for a mixed initial state. Sometimes the probability is characterized by projector to “out state” $|\psi_{\text{out}}\rangle$ [2, 10] and in such a case $\hat{M}_{\text{out}} = |\psi_{\text{out}}\rangle\langle\psi_{\text{out}}|$ may be used in Eq. 56 producing an equivalent expression $p = |\langle\psi_{\text{out}}|\hat{\mathcal{U}}|\psi_{\text{in}}\rangle|^2$, but more general \hat{M}_{out} is considered here

to take into account an alternative approach [7, 8] and methods discussed below.

Let us consider for modeling of a qubit chain initial states $|j\rangle$ Eq. 6 and measurement operators

$$\hat{M}_k \equiv \hat{n}_k^z = \frac{\hat{I} - \hat{\sigma}_k^z}{2} = \hat{a}_k^\dagger \hat{a}_k. \quad (57)$$

With the operator \hat{M}_k the probability to find the unit at the node k for the initial state $|j\rangle$ may be found using Eq. 56 and Eq. 57

$$\begin{aligned} p_{j \rightarrow k} &= \langle j | \hat{U}^\dagger \hat{a}_k^\dagger \hat{a}_k \hat{U} | j \rangle = \langle j | \hat{U}^\dagger \hat{a}_k^\dagger \hat{U} \hat{U}^\dagger \hat{a}_k \hat{U} | j \rangle \\ &= \sum_{l,r} \langle j | \bar{U}_{kl}^* \hat{a}_l^\dagger \mathbf{U}_{kr}^* \hat{a}_r | j \rangle = \sum_{l,r} \mathbf{U}_{lk} \bar{U}_{rk} \langle j | \hat{a}_l^\dagger \hat{a}_r | j \rangle \\ &= \sum_l |\mathbf{U}_{lk}|^2 \langle j | \hat{a}_l^\dagger \hat{a}_l | j \rangle = |\mathbf{U}_{jk}|^2. \end{aligned} \quad (58)$$

The evolution of states $|j\rangle$ can be described more directly due to yet another approach also used in [2]. Let us denote

$$|\emptyset\rangle \equiv |\underbrace{0 \dots 0}_n\rangle. \quad (59)$$

Creation operators \hat{a}_k^\dagger defined in Eq. 47 for the representation Eq. 30 meet the natural condition

$$|\underline{k}\rangle = \hat{a}_k^\dagger |\emptyset\rangle. \quad (60)$$

Any admissible evolution conserves the number of units in the computation basis and so

$$\hat{U} |\emptyset\rangle = |\emptyset\rangle. \quad (61)$$

Using such properties it may be written

$$\begin{aligned} \hat{U} |\underline{k}\rangle &= \hat{U} \hat{a}_k^\dagger |\emptyset\rangle = \hat{U} \hat{a}_k^\dagger \hat{U}^\dagger \hat{U} |\emptyset\rangle \\ &= \sum_{j=1}^n \bar{U}_{kj} \hat{a}_j^\dagger |\emptyset\rangle = \sum_{j=1}^n \bar{U}_{kj} |j\rangle = \sum_{j=1}^n \mathbf{U}_{jk}^\dagger |j\rangle. \end{aligned} \quad (62)$$

For a state $|\psi\rangle$ defined as a linear superposition of $|\underline{k}\rangle$

$$\hat{U} |\psi\rangle = \sum_{k=1}^n \psi_k \hat{U} |\underline{k}\rangle = \sum_{j,k=1}^n \mathbf{U}_{jk}^\dagger \psi_k |j\rangle \equiv \sum_{j=1}^n \psi'_j |j\rangle, \quad \psi'_j = \sum_{k=1}^n \mathbf{U}_{jk}^\dagger \psi_k. \quad (63)$$

Formally, the Eq. 63 produces a correspondence with the unitary evolution \mathbf{U}^\dagger of a scalar chain with n nodes considered earlier. It has some similarity with the approach used for the perfect state transfer for particular Hamiltonians Eq. 8 or Eq. 10 of a higher-spin system. However, \mathbf{U} in Eq. 54 is an arbitrary $n \times n$ unitary matrix and the evolution of state $|\underline{\psi}\rangle$ due to Eq. 63 can be considered for many different kinds of quantum chains with required properties.

The simulation of the measurement for a qubit chain in single-particle is effective, because the evolution is limited by n -dimensional span of states $|k\rangle$ Eq. 6 and a scalar chain with n nodes can be used instead as a model without lost of generality. Such a correspondence also clarifies Eq. 58 derived earlier less directly.

5.2 Multi-particle simulation

Rather straightforward transition to the consideration of an evolution with many particles is an essential property of the qubit chain model considered here. The general scheme from [2, 7, 8, 10] is again appropriate for such a purpose.

The generalization of a single-particle configuration Eq. 60 is a basic state

$$|\underline{K}\rangle \equiv |k_1, \dots, k_m\rangle = \hat{a}_{k_1}^\dagger \cdots \hat{a}_{k_m}^\dagger |\underline{\emptyset}\rangle \quad (64)$$

with m units in positions $k_1 < \dots < k_m$. For example, an analogue of Eq. 6 with *two neighboring* particles is

$$|\underline{k, k+1}\rangle \equiv \underbrace{|0 \dots 0}_{k-1} 11 \underbrace{0 \dots 0}_{n-k-1}\rangle = \hat{a}_k^\dagger \hat{a}_{k+1}^\dagger |\underline{\emptyset}\rangle. \quad (65)$$

Let us denote

$$\hat{a}_k^u = \hat{\mathcal{U}} \hat{a}_k \hat{\mathcal{U}}^\dagger = \sum_l \mathbf{U}_{kl} \hat{a}_l \quad (66)$$

with the obvious property $\hat{a}_k^u \hat{a}_l^u = -\hat{a}_l^u \hat{a}_k^u$. For the initial states Eq. 64 taking into account Eq. 61

$$\hat{\mathcal{U}}|\underline{K}\rangle = \hat{\mathcal{U}}|k_1, \dots, k_m\rangle = \hat{\mathcal{U}} \hat{a}_{k_1}^\dagger \hat{\mathcal{U}}^\dagger \cdots \hat{\mathcal{U}} \hat{a}_{k_m}^\dagger \hat{\mathcal{U}}^\dagger \hat{\mathcal{U}} |\underline{\emptyset}\rangle = \hat{a}_{k_1}^{u\dagger} \cdots \hat{a}_{k_m}^{u\dagger} |\underline{\emptyset}\rangle. \quad (67)$$

The evolution is represented as the *antisymmetric product* of operators $\hat{a}_k^{u\dagger}$ generating distributions Eq. 62 for particles in different initial positions. Such

representation should be considered rather as some model *without interaction*.

Indeed, let us associate with any single-particle state $|\underline{\psi}\rangle$ Eq. 44 an operator

$$\hat{\psi} \equiv \sum_{k=1}^n \psi_k \hat{a}_k^\dagger, \quad \hat{\psi}|\underline{\emptyset}\rangle = |\underline{\psi}\rangle. \quad (68)$$

For the two-particle case the composition of such operators correspond to an anti-symmetric (exterior) product defined on n -dimensional single-particle space

$$\hat{\psi}\hat{\phi}|\underline{\emptyset}\rangle = |\underline{\psi}\rangle \wedge |\underline{\phi}\rangle. \quad (69)$$

It follows directly from the antisymmetry of creation operators and the formal definition of the exterior product [39, 40] for the basic states

$$|\underline{j}, \underline{k}\rangle \equiv |\underline{j}\rangle \wedge |\underline{k}\rangle = -|\underline{k}\rangle \wedge |\underline{j}\rangle \quad (j < k), \quad |\underline{j}\rangle \wedge |\underline{j}\rangle = 0. \quad (70)$$

The generalization to the multi-particle space is straightforward and the evolution Eq. 67 may be rewritten now as an exterior product of single-particle terms

$$\hat{\mathcal{U}}|\underline{K}\rangle = \hat{\mathcal{U}}|\underline{k}_1, \dots, \underline{k}_m\rangle = \hat{\mathcal{U}}|\underline{k}_1\rangle \wedge \dots \wedge \hat{\mathcal{U}}|\underline{k}_m\rangle. \quad (71)$$

It was already shown above, that each single-particle term in Eq. 71 evolution can be modeled by an operator \mathbf{U}^\dagger on a simple chain with n nodes. Thus, the multi-particle evolution corresponds to the anti-symmetric product of m such chains.

An effective simulation of the evolution together with the measurement may require additional efforts if the number of particles is large. Some general methods developed for the description of match-circuits may be found elsewhere [2, 3, 7, 8, 9, 10] and the *restricted case* is relevant here for the *admissible evolution* with creation and annihilation operators and it was also already discussed earlier by different authors [2, 10].

Methods of simulation depend on the scheme of the initialization and the measurement. For the many problem of the quantum state distribution an initial state may be chosen from the computational basis. The output of the simulation may use an approach from [8] with the measurement in the computational basis. In such a case the probability of the ‘‘occupation’’ (unit) for any node k may be effectively calculated using a simplified approach discussed in [7, 8].

Let us write an analogue of Eq. 58 for the probability to find a particle on the node k after the evolution of the multi-particle state Eq. 64

$$\begin{aligned}
p_{K \rightarrow k} &= \langle \underline{K} | \hat{U}^\dagger \hat{a}_k^\dagger \hat{a}_k \hat{U} | \underline{K} \rangle = \sum_{l,r} \mathbf{U}_{lk} \bar{\mathbf{U}}_{rk} \langle \underline{K} | \hat{a}_l^\dagger \hat{a}_r | \underline{K} \rangle \\
&= \sum_l |\mathbf{U}_{lk}|^2 \langle \underline{K} | \hat{a}_l^\dagger \hat{a}_l | \underline{K} \rangle = \sum_{l \in K} |\mathbf{U}_{lk}|^2.
\end{aligned} \tag{72}$$

In the more general case such approach with the separate measurements of a qubits could be not enough to uncover some nontrivial quantum correlations between qubits. Measurements of multi-qubit output would require more complicated methods for effective classical simulations [2, 10]. However, the multi-particle case for given model has the understanding exterior structure Eq. 71 and more general measurement schemes are not discussed here.

6 Conclusion

The application of a particular non-universal set of quantum gates and Hamiltonians was discussed in this work. Different examples of the state distribution along a chain of qubits was investigated for such a purpose.

A single particle on a chain is a convenient simplified model and it is used for the comparison of scalar and qubit chains in Sect. 3. An arbitrary unitary operator on a scalar chain can be associated with some effectively modeled evolution of a qubit chain using methods from Sect. 4.3. For the multi-particle case an evolution of a qubit chain for the considered model is mapped in Sect. 5.2 into the anti-symmetric product of such a scalar chains.

The certain difficulty of the considered approach is a lack of the simple possibility for a generalization of the methods for effective modeling from a chain on arbitrary graph, because linked nodes may not always correspond to consequent indexes. For a qubit ring the similar approach still may work efficiently [10], but the discussion about more general graphs falls outside the limits of presented work.

Acknowledgements

The author is grateful to anonymous referees for corrections and suggestions to initial version of the article.

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