Simulating Hamiltonians in Quantum Networks: Efficient Schemes and Complexity Bounds

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Abstract

We address the problem of simulating pair-interaction Hamiltonians in n node quantum networks where the subsystems have arbitrary, possibly different, dimensions. We show that any pair-interaction can be used to simulate any other by applying sequences of appropriate local control sequences. Efficient schemes for decoupling and time reversal can be constructed from *orthogonal arrays*. Conditions on time optimal simulation are formulated in terms of *spectral majorization* of matrices characterizing the coupling parameters. Moreover, we consider a specific system of n harmonic oscillators with bilinear interaction. In this case, decoupling can efficiently be achieved using the combinatorial concept of *difference schemes*. For this type of interactions we present optimal schemes for inversion.

1 Introduction

The conjecture that quantum computers might be able to simulate the time evolution of quantum systems better than classical computers has already been stated in [8]. Various schemes for constructing gate sequences which simulate the unitary evolution corresponding to a given Hamiltonian have been suggested (see e. g. [18, 23]). More recently, a quite different approach to this problem has become popular: considering the quantum computer as a quantum system with Hamiltonian evolution as well, a *simulation* is a sequence of control operations acting on the quantum computer in such a way that the net effect is a time evolution analogous to the evolution of the system we want to simulate [6, 27, 12, 1, 25, 20]. In the setting described in the following the simulation problem can be stated in a control-theoretical fashion. Assume that the total quantum system is a quantum network, i. e., a system consisting of n subsystems. The Hilbert space is the tensor product

$$\mathcal{H} := \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_n \,,$$

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where[1] $\mathcal{H}_j := \mathbb{C}^d$ for $j = 1, \ldots, n$ and $d \in \mathbb{N}$. Let $\{\sigma_\alpha \mid \alpha = 1, \ldots, d^2 - 1 =: m\}$ be an orthogonal basis of the $\mathbb{R}$-vector space $su(d)$ of traceless Hermitian operators on $\mathbb{C}^d$. We assume that both the Hamiltonian to be simulated and the Hamiltonian H of the system are sum of pair-interactions between nodes and free evolutions on each individual node. Hence the system Hamiltonian is given by

$$H := \sum_{kl;\alpha\beta} J_{kl;\alpha\beta} \sigma_\alpha^k \sigma_\beta^l + \sum_{k;\alpha} r_{k;\alpha} \sigma_\alpha^k \,, \tag{1}$$

where J is a real symmetric $mn \times mn$-matrix and r is an mn-dimensional real vector. Furthermore, we assume that the only transformations which can be implemented directly by external control interactions are local transformations of the form

$$U := V_1 \otimes V_2 \otimes \cdots \otimes V_n \,, \tag{2}$$

where each V_j for $j = 1, \ldots, n$ is an element of the special unitary group $SU(d)$. Assuming that the implementations of V_j are fast compared to the natural evolution given by H ("fast control limit"), the time evolution according to $U^\dagger H U$ can be simulated by alternating the natural time evolution with implementations of $U^\dagger$ and U. Here we make use of the identity

$$U^\dagger \exp(-iHt) U = \exp(-iU^\dagger H U t) \,.$$

Concatenating the unitary transformations $\exp(-iU_j^\dagger H U_j \tau_j)$ we obtain an approximation of the time evolution corresponding to the "average Hamiltonian"

$$\tilde{H} := \frac{1}{\sum_j \tau_j} \sum_j \tau_j U_j^\dagger H U_j \,,$$

if the times τ_j are assumed to be sufficiently small (for details see [7])[2]. In this sense, the set of Hamiltonians which can be simulated with no time overhead is exactly the *convex span* of the set $\mathcal{S} := \{U^\dagger H U\}$, where U is as in eq. (2). For a formal definition of the notion of time overhead of a simulation see [27, 1]. Intuitively, if the only possibility to write a Hamiltonian as a positive linear combination of elements of the form $UHU^\dagger$ is to do it in such a way that the sum of the coefficients is greater than one, then the sum of these coefficients is precisely the *time overhead* of the simulation. A suitably *rescaled* Hamiltonian is then in the convex span of $\mathcal{S}$. As noted in [27, 1], the minimal overhead for simulating a Hamiltonian $\tilde{H}$ by the physical Hamiltonian H is the smallest positive τ such that $\tilde{H}/\tau$ is in the convex span of $\mathcal{S}$.

Note that convex problems of this kind are closely related to the method for obtaining pseudopure states by averaging over random unitary transformations [16]. Pseudopure states are states that can be written as convex combination of the maximally mixed state (with density matrix $\mathbf{1}/d$) and a pure state $|\psi\rangle\langle\psi|$. Writing a general state as $\rho = \mathbf{1}/d + A$, where A is the traceless part, we have that ρ can be transformed into the pseudopure state $(1-\lambda)\mathbf{1}/d + \lambda|\psi\rangle\langle\psi|$ by averaging over unitary transformations

[1] For reasons of convenience of notation we assume that the subsystems have equal dimensions. However, note that our results on universal simulations generalize straightforwardly to arbitrary dimensions.

[2] Note that an approach of this kind is generally accepted for describing Nuclear Magnetic Resonance experiments.

if and only if A can be transformed (without time overhead) into the traceless operator $-\lambda\mathbf{1}/d + \lambda|\psi\rangle\langle\psi|$. Determining the optimal *signal-to-noise ratio* of the attainable pseudopure state is hence directly related to determining minimal time overhead of simulation schemes.

For an arbitrary interaction between two qubits, minimization of the time overhead has been carried out in [1]. In case of n qubits and pair-interaction Hamiltonians H and $\tilde{H}$ the situation is more complicated: the problem of optimal simulation of $\tilde{H}$ by H cannot be reduced to the two-qubit case. The difficulty arising here is that the required operations on qubit k for simulating an interaction between qubit k and l might not coincide with the required operations on k for simulating another interaction between k and m. The fact that the control operations for simulating interactions between non-disjoint qubit pairs must be consistent on the common qubit seems to be a highly non-trivial combinatorial problem. Some upper and lower bounds for the time overhead are given in [12, 27].

The issue of optimal simulation has consequences for the problem to parallelize operations of discrete quantum algorithms. The maximal degree of parallelization is constrained since a given interaction may allow to implement concatenations of some two-qubit gates even if they act on *non-disjoint* qubit pairs. Assume for instance that a Hamiltonian on three qubits is given by

$$H := \sigma_z \otimes \sigma_z \otimes 1 + \sigma_z \otimes 1 \otimes \sigma_z + 1 \otimes \sigma_z \otimes \sigma_z,$$

where σ_z denotes the Pauli matrix. Then, for generic times $t > 0$, the unitary $\exp(-iHt)$ is a concatenation of three two-qubit gates, which can be implemented "simultaneously" by waiting the time t. But there is no obvious way for such a fast implementation of $\exp(-iHt)$ for *negative* t provided that H is the system Hamiltonian. One can even show that there exist negative values of t such that the implementation of $\exp(-iHt)$ cannot be performed in principle within a time period of length $|t|$, since H is not able to simulate $-H$ without time overhead [12]. For n qubits with $\sigma_z \otimes \sigma_z$-interactions the minimal overhead is known to be at least $n-1$. This shows that the question of optimal parallelism of sequences of gates is rather sensitive to the form of the underlying Hamiltonian. Hence the question of optimal implementation of complex transformations on an n-partite system cannot be answered alone by resolving the network into elementary gates: the question of maximally possible parallelism appears already on the control-theoretic level.

The paper is organized as follows. In Section 2 we construct decoupling schemes from orthogonal arrays. Selective decoupling can be achieved by straightforward generalizations. Therefore each pair-interaction Hamiltonian on an n-partite systems can be converted into any other provided that a sufficient set of local unitary control operations is available (the so-called *transformer groups* introduced in [28]). Such a simulation has time overhead of $O(n^2)$. Our schemes works even if the dimensions of the n subsystems do not agree, thereby solving a problem stated in [20].

A *lower* bound on the time complexity of mutual simulation of different Hamiltonians is shown which uses the spectra of matrices describing the coupling parameters of the interaction. Efficient schemes for switching off all the interactions ("decoupling schemes") are constructed. Using the combinatorial concept of *orthogonal arrays* decoupling can be achieved if local transformations of a unitary error basis are available.

The length of the required sequence of local transformations grows linearly with the number of nodes.

A specific form of interactions is dealt with in Section 3. There we consider harmonic oscillators coupled by bilinear terms of creation and annihilation operators. In this case rather simple decoupling schemes can be constructed on the basis of *difference schemes*, another concept from combinatorics. Furthermore we discuss the generalization of this problem where a given bilinear interaction is used to simulate another interaction of this form with different coupling parameters. Finding the time optimal simulation is equivalent to the mathematical problem of constructing vectors of minimal length with complex entries of modulus one such that their inner products yield certain values. This fact is used for deriving a lower bound on the simulation time. In contrast to the general system Hamiltonian, the *upper* bound is $O(n)$. An optimal scheme for time inversion is constructed.

In Section 4 we discuss the connection between the decoupling schemes of Section 2 and the schemes presented in [17].

2 Simulating Hamiltonians in Networks

2.1 Selective Decoupling

A useful tool for simulating Hamiltonians in multi node quantum networks is given by decoupling schemes, i. e., sequences of local operations which switch off unwanted interactions. First we describe schemes for decoupling all the interactions. Schemes for decoupling two interacting quantum systems—mainly in the context of a quantum register which is coupled to a bath—have been derived in [26, 29]). Decoupling of n-partite systems interacting with each other by two-body Hamiltonians has been considered in [17, 24] for the case of qubits. In [20] it was noted that decoupling of bipartite systems can be concatenated in such a way that the system is separated into suitable clusters of subsystems without coupling between different clusters. The number of operations involved in this scheme is $O(n^{2\log_2 d})$. In this paper we present a construction based on orthogonal arrays which uses $O(n)$ operations provided that the dimension d of the nodes is a prime power.

Straightforward generalizations of decoupling schemes allow to switch off all interactions except the Hamiltonian of a pair of nodes ("selective recoupling") or the Hamiltonian of a single node. We have shown in [28] that any bipartite Hamiltonian can simulate any other provided that it consists of non-trivial local Hamiltonians on both nodes and a non-trivial coupling. If this criterion is met by all pairs of an n-partite Hamiltonian then universal simulation of all pair-interaction Hamiltonians is possible[3]. This result is also true if not every local operation is available, it is sufficient that all the elements of a so-called *transformer group* (a concept introduced in [28]) can be implemented. The simulation time overhead is of order $O(n^2)$ since there are $n(n-1)/2$ pairs of nodes.

Rephrasing well-known results about decoupling (e. g. [26, 29]) in our language, we

[3]Note that the condition that *all* the couplings have to be non-trivial is only necessary in the average Hamiltonian approach. If higher order terms in the time interval are considered interactions between nodes k and l resp. k and m can be used for simulating a coupling between l and m as noted in [6, 20].

briefly describe decoupling for bipartite systems. Remember that the Hamiltonian on a d-dimensional quantum system can be cancelled if an appropriate sequence of unitary control operations is applied [28].

Definition 1 (Annihilator) *An annihilator* $A := (U_1, \tau_1, U_2, \tau_2, \ldots, U_N, \tau_N)$ *of dimension* d *and length* N *is given by unitaries* $U_i \in SU(d)$ *and relative times* $\tau_i > 0$, $\sum_{i=1}^{N} \tau_i = 1$ *such that*

$$\sum_{i=1}^{N} \tau_i U_i^\dagger a U_i = 0$$

for all $a \in su(d)$. *An annihilator is called minimal if there is no shorter annihilator.*

A minimal annihilator of dimension d has length d^2 (as already noted in [26] and proved in [28]) and all τ_i are equal. Moreover, the unitaries U_i must form a *unitary error basis* of operators in $\mathbb{C}^{d\times d}$, i. e. a collection of d^2 unitaries U_i that are orthogonal with respect to the trace inner product $\langle A|B\rangle := \mathrm{tr}(A^\dagger B)/d$. Such unitaries can be explicitly constructed using nice error bases [15, 14].

Being a special case of equation (1) we write the general Hamiltonian of a bipartite system as follows:

$$H = \sum_{\alpha\beta} J_{\alpha\beta}\, \sigma_\alpha \otimes \sigma_\beta + \sum_{\gamma} r_\gamma\, \mathbf{1} \otimes \sigma_\gamma + \sum_{\delta} s_\delta\, \sigma_\delta \otimes \mathbf{1}\,. \tag{3}$$

Let $\mathcal{E}_1 = \{U_i\}$ and $\mathcal{E}_2 = \{V_i\}$ be unitary error bases of the respective systems and let $\mathcal{A}$ denote the set $\{1, \ldots, d^2\}$. By applying the annihilators defined by $\mathcal{E}_1$ and $\mathcal{E}_2$ independently on the nodes we can switch off the Hamiltonian, i. e.

$$\frac{1}{|\mathcal{A}^2|} \sum_{(i,j)\in\mathcal{A}^2} (U_i^\dagger \otimes V_j^\dagger)\, H\, (U_i \otimes V_j) = 0\,. \tag{4}$$

We describe a decoupling scheme on n nodes by n unitary error basis $\mathcal{E}_1, \ldots, \mathcal{E}_n$ and an $n \times N$-matrix $M = (m_{ij})_{i=1,\ldots,n, j=1,\ldots,N}$. This matrix contains elements of $\mathcal{A}$ specifying the conjugation by the m_{ij}^{th} unitary of $\mathcal{E}_i$ on a specific node i for a certain time interval j. The N time intervals correspond to the columns and the different nodes correspond to different rows. For instance the decoupling scheme corresponding to (4) is given by the array

$$\left(\begin{array}{cccc|cccc|c|cccc} 1 & 1 & \ldots & 1 & 2 & 2 & \ldots & 2 & \ldots & N & N & \ldots & N \\ 1 & 2 & \ldots & N & 1 & 2 & \ldots & N & \ldots & 1 & 2 & \ldots & N \end{array}\right) \tag{5}$$

and unitary error bases $\mathcal{E}_1 = \{U_i\}$ and $\mathcal{E}_2 = \{V_i\}$ corresponding to the first and second node, respectively.

The simplest approach for decoupling is to choose the columns of M as all tuples of $\mathcal{A}^n$. However, this scheme is not efficient in terms of the number of time intervals and pulses since both scale exponentially as d^{2n} because the sequence has to be repeated d^2 times for each added node.

More efficient schemes can be constructed using the combinatorial structure of orthogonal arrays. See [2, 5, 9] for the general theory of orthogonal arrays. Orthogonal

arrays have numerous applications e. g., in the design of experiments. Also there are connections between orthogonal arrays and mutually orthogonal Latin squares and transversal designs (cf. [2, Section VIII]). The following definition takes account of the fact that for purposes of decoupling we need a special type of orthogonal arrays, namely those of strength $t = 2$ (cf. [2, 5, 9] for the general case). Also the notation used is adapted to this situation.

Definition 2 *Let $\mathcal{A}$ be a finite alphabet and let $n, N \in \mathbb{N}$. An $n \times N$ array M with entries from $\mathcal{A}$ is an orthogonal array with $|\mathcal{A}|$ levels, strength $t = 2$, and index λ if and only if each pair of elements of $\mathcal{A}$ occurs λ times in the list $((m_{kj}, m_{lj}) \mid j = 1, \dots N)$ for $1 \leq k < l \leq n$. We use the notation $OA_\lambda(n, N)$ to denote a corresponding orthogonal array.*[4]

The following theorem shows that decoupling in networks of arbitrary dimensions can be achieved using pulse sequences obtained by orthogonal arrays.

Theorem 1 (Decoupling) *Let $\mathcal{A}$ be the finite alphabet $\{1, \dots, d^2\}$. Then any orthogonal array with parameters $OA_\lambda(n, N)$ over $\mathcal{A}$ can be used to decouple a quantum network consisting of n nodes of dimension d. The number of local operations used in this scheme is given by N.*

Proof: Let $M = (m_{ij})$ be an $n \times N$-matrix over $\mathcal{A}$ corresponding to the parameters $OA(n, N)$. Choose unitary error bases $\mathcal{E}_1, \dots, \mathcal{E}_n$ where $\mathcal{E}_k = \{E_i^k : i = 1, \dots, d^2\}$ to define annihilators for each node. For each row k of M let $(E_{m_{k,j}}^k : j = 1, \dots, N)$ be the corresponding local conjugations on node k. We now consider a pair of nodes, i. e., two rows k and l of M, and show that the local terms and the coupling between the two nodes are switched off. Since each pair of elements of $\mathcal{A}$ occurs precisely λ times in the list $((m_{kj}, m_{lj}) \mid j = 1, \dots, N)$ the averaged Hamiltonian $H_{k,l}$ on the nodes k and l is given by (setting $U_i := E_i^k$ and $V_i := E_i^l$)

$$\frac{1}{|\mathcal{A}^2|} \sum_{(i,j) \in \mathcal{A}^2} (U_i^\dagger \otimes V_j^\dagger)\, H_{k,l}\, (U_i \otimes V_j).$$

This sum is equal to zero since both annihilators are applied independently on both nodes. □

For any given number $n \in \mathbb{N}$ of nodes there are parameters λ, N such that an orthogonal array $OA(n, N)$ exists. However, since we are interested in efficient schemes, N has to be a polynomial in the number n of nodes. Also it is of interest to give explicit constructions of such schemes, i. .e, of orthogonal arrays. Whereas little is known about the existence of efficient schemes for general n and alphabet size $s := |\mathcal{A}|$ the situation is much better in the case when s is a prime power.

Corollary 1 *Let an n-node quantum network with pair-interaction Hamiltonian be given and let the dimension d of each node be a prime power. Then there exists a decoupling scheme using N local operations, where $N \leq cn$ and c is a constant depending only on d.*

[4]Note that in [2] the notation $OA_\lambda(n, s)$ is used for an orthogonal array with $N = \lambda s^2$ in our notation, where $s := |\mathcal{A}|$.

Proof: Let $s := d^2$ be the size of a minimal annihilator for a d-dimensional system. In view of Theorem 1 we have to show that there exists an orthogonal array with parameters $OA_\lambda(\tilde{n}, N)$ with $n \leq \tilde{n}$ and $N \leq cn$ as above. The result [9, Theorem 3.20] gives an explicit construction for an $OA((s^i - 1)/(s - 1), s^i)$ for any $i \geq 2$. Hence, if for the number of nodes $n = (s^i - 1)/(s - 1)$ holds, we have found a decoupling scheme with $N = s^i = (s - 1)n + 1$ operations, i. e., $N = O(n)$. For general n we embed into an OA of this form. Switching to the next number of the form $(s^i - 1)/(s - 1)$ with suitable $i \geq 1$ can be achieved be multiplying n with a number less or equal s, i. e., $\tilde{n} \leq sn$. □

Remark 1 *There are tables of OAs covering the small instances (cf. [2, 5, 9]). We remark that there is a family of OAs with parameters* $OA(2s^i, 2\frac{s^i-1}{s-1} - 1)$ *[9, Theorem 6.28]. This shows that the constant c in Corollary 1 can be improved to* $c/2$.

The following example illustrates that OAs give more efficient schemes already for small systems.

Example 2 *We consider the case of four three-level systems. Using the exponential scheme we need* $s^4 = 6561$ *local operations to decouple all interactions. Following 1 we obtain a decoupling scheme with the same property that uses only* $s^2 = 81$ *local operations.*

Selective decoupling can be achieved as follows. If the decoupling scheme is applied to all but one or two nodes, the remaining Hamiltonian is the local Hamiltonian of the node or the bipartite Hamiltonian of the two nodes, respectively.

The assumption that every node is coupled to all the other nodes is too strong in many physical systems since many coupling terms might be neglected. This reduces the overhead for decoupling and inverting the time evolution.

In general the interaction graph of a partially coupled network is a non-complete graph. Each graph can be colored, by assigning each vertex one of a number of different colors. Such a coloring scheme is called a *proper* coloring if no two connected vertices have the same color. The chromatic number χ is the smallest number of colors required to properly color the graph. In a complete graph (a fully coupled network) $\chi = n$, but in a partially coupled network the chromatic number can be much smaller. This observation permits to derive more efficient decoupling schemes [13] since if the network is represented by a properly colored graph, then there are no constraints on the pulse sequences between nodes with the same color. It is sufficient to create a decoupling scheme of a completely coupled χ-node network, and apply identical sequences to all nodes of the same color.

Note that the selective decoupling scheme presented above generalize straightforwardly to the case that the dimensions of the n subsystems do not agree. Then one has to use so-called *mixed orthogonal arrays*, i. e., one has different alphabets $\mathcal{A}$ for different nodes. Although little is known about constructions of efficient mixed orthogonal arrays, it is known that exponential ones exist (cf. [9, Section 9.3]). Furthermore, the mutual simulation of Hamiltonians on bipartite systems is also possible for different dimensions, since the proof in [28] does only rely on the fact that on each of the subsystems (possibly different) transformer groups are available.

2.2 Lower bound on the simulation time overhead

In order to derive lower bounds on the overhead for the simulation time we neglect the free evolution and consider the weaker problem to simulate the desired Hamiltonian on n nodes up to local terms of each node. Note that the local terms become irrelevant when allowing arbitrary unitary operations on the nodes.

In the following it will be convenient to represent the interaction Hamiltonian by the so-called J-matrix

$$J = \begin{pmatrix} 0 & J_{12} & J_{13} & \cdots & J_{1n} \\ J_{21} & 0 & J_{23} & \cdots & J_{2n} \\ J_{31} & J_{32} & 0 & & J_{3n} \\ \vdots & \vdots & & \ddots & \\ J_{n1} & J_{n2} & J_{n3} & & 0 \end{pmatrix} \in \mathbb{R}^{mn \times mn}, \tag{6}$$

where the matrix J_{kl} describes the coupling between the nodes k and l and J_{lk} is the transpose of J_{kl} in eq. (1).

Let H and $\tilde{H}$ be arbitrary pair-interaction Hamiltonians. We investigate the question whether $\tilde{H}$ can be simulated by H with overhead τ. This defines a quasi-order of the pair-interaction Hamiltonians for $\tau = 1$. A partial characterization of the quasi-order is expressed in terms of majorization of the spectra of the corresponding matrices J and $\tilde{J}$. Note that this criterion does not coincide with the criterion given in [1] for two qubits since the latter refers to the spectrum of the Hamiltonians and not of the J-matrices. To make this more precise we introduce the following notation. Let $x = (x_1, \ldots, x_d)$ and $y = (y_1, \ldots, y_d)$ be two d-dimensional real vectors. We introduce the notation $\downarrow$ to denote the components of a vector rearranged into non-increasing order, so $x^{\downarrow} = (x_1^{\downarrow}, \ldots, x_d^{\downarrow})$, where $(x_1^{\downarrow} \geq x_2^{\downarrow} \geq \ldots \geq x_d^{\downarrow})$. We say that x is majorized by y and write $x \prec y$, if

$$\sum_{j=1}^{k} x_j^{\downarrow} \leq \sum_{j=1}^{k} y_j^{\downarrow},$$

for $k = 1, \ldots, d-1$, and $\sum_{j=1}^{d} x_j^{\downarrow} = \sum_{j=1}^{d} y_j^{\downarrow}$ (see [3]). The usefulness of majorization techniques in quantum information processing has first been demonstrated in [19] in the context of transforming states under local operations and classical communication. In [27] majorization was used in the context of simulation of Hamiltonians in quantum networks of qubits.

Let $\mathrm{Spec}(X)$ denote the spectrum of the Hermitian matrix X, i. e. the vector of eigenvalues. Ky Fan's maximum principle [3] gives rise to a useful constraint on the eigenvalues of a sum $C := A + B$ of two Hermitian matrices:

$$\mathrm{Spec}(A + B) \prec \mathrm{Spec}(A) + \mathrm{Spec}(B). \tag{7}$$

Based on these tools we derive the following bound, which generalizes the bounds given in [27] from qubits to qudits. The second statement of the theorem even tightens the bound for qubits given there.

Theorem 3 (Lower bound) *Let H and $\tilde{H}$ be arbitrary pair-interaction Hamiltonians. A necessary condition that $\tilde{H}$ can be simulated with overhead τ by H is that the spectrum of $\tilde{J}$ is majorized by the spectrum of τJ. Furthermore it is necessary*

that this majorization criterion is still satisfied after rescaling the couplings as follows: $J'_{kl} := s_{kl}J_{kl}$ *and* $\tilde{J}' := s_{kl}\tilde{J}$*, where* $S = (s_{kl})$ *is an arbitrary real symmetric* $n \times n$*-matrix.*

Proof: We choose an orthonormal basis B (with respect to the trace inner product) for $su(d)$. Each $a \in su(d)$ can be represented by $|a\rangle = (tr(a\sigma_1), \dots tr(a\sigma_{d^2-1}))^T$ with $\sigma_i \in B$. Conjugation of $a \in su(d)$ by a unitary $u \in SU(d)$ corresponds to an element of $SO(d^2-1)$ rotation of $|a\rangle$. The subgroup of $SO(d^2-1)$ defined by the adjoint action of $SU(d)$ in this way will be denoted by $\mathcal{R}$.

Representing the Hamiltonians H and $\tilde{H}$ by their J matrices we see that $\tilde{H}$ can be simulated with overhead τ if and only if there is a sequence of special orthogonal matrices $U_j = U_{j1} \oplus U_{j2} \oplus \cdots \oplus U_{jn}$, where $U_{j,k} \in \mathcal{R}$ for all j, k and $\tau_i > 0$ with $\sum_j \tau_j = \tau$ such that

$$\tilde{J} = \sum_j \tau_j U_j J U_j^T \,. \tag{8}$$

The proof now follows from Uhlmanns's theorem [21] which implies that spectrum $\tilde{J}$ is majorized by the spectrum of τJ.

The second statement is a direct consequence from the first one since the same simulation procedure can be used for the rescaled problem. □

Note that for $d > 2$ not every rotation in $SO(d^2-1)$ corresponds to a conjugation by a unitary in $SU(d)$. Therefore this condition seems to be the weaker the greater d gets. A necessary condition for the fact that H can simulate $\tilde{H}$ with overhead τ is that $\mathrm{Spec}(\tilde{H}) \prec \tau\mathrm{Spec}(H)$, i. e. a condition based on majorization of the spectra of the Hamiltonians. Clearly the size of the matrices representing the Hamiltonians grows exponentially with n, whereas the size of their J-matrices grows only linearly with n. This makes the J-representation useful for calculations. Furthermore, in some important cases it permits to derive tight bounds (see Section 3 and [12]).

2.3 Inverting

We now consider the problem to invert an arbitrary, possibly unknown Hamiltonian in a quantum network, i. e. to simulate $-H$ when H is present. It is well-known that this question is closely related to the construction of decoupling schemes (e. g. [22, 26, 17]). Lower bounds on the time overhead for time-reversal in n-qubit systems were given in [12]. In the case of a single node we can invert the time evolution by summing over all elements of the unitary error basis but the identity. This trick can be generalized to the case of multiple nodes. For that we introduce the notion of *normal form* for decoupling schemes.

Definition 3 (Normal form) *Let* $\mathcal{O}$ *be an* $OA_\lambda(n, N)$*. Assume in addition that the alphabet* $\mathcal{A}$ *consists of the elements of a finite group* G*. We say that* $\mathcal{O}$ *is in normal form if each entry in the first column of* $\mathcal{O}$ *is the identity element of* G*.*

Lemma 1 *Let* $\mathcal{O}$ *be an* $OA_\lambda(n, N)$*. Then there is an orthogonal array with the same parameters which is in normal form.*

Proof: We identify the underlying alphabet $\mathcal{A}$ with an arbitrary finite group G of order $|\mathcal{A}|$. Consider two rows $(g_1, \ldots, g_N)$ and $(h_1, \ldots, h_N)$ of $\mathcal{O}$. Multiplying the elements of the rows by g_1^{-1} and h_1^{-1} respectively preserves the property that all pairs occur with frequency λ since $G \times G$ is invariant under multiplication by fixed elements. □

Based on the normal form of OAs we now give an inversion scheme for a general, possibly unknown pair-interaction Hamiltonian.

Theorem 4 (Inverting) *Any $OA(n, N)$ can be used to invert the time evolution of a quantum network consisting of n nodes. The number of local operations used is $N - 1$ and the time overhead is $N - 1$.*

Proof: By Lemma 1 we assume that the orthogonal array $\mathcal{O}$ is in normal form and M is the corresponding $n \times N$ matrix over the alphabet $\mathcal{A}$ which in turn is identified with the elements of a finite group G. Furthermore, we choose unitary error bases $\mathcal{E}_1, \ldots, \mathcal{E}_n$ where $\mathcal{E}_k = \{E_i^k : i = 1, \ldots, d^2\}$ and identify the identity element of G with the corresponding identity matrices. For any pair k, l of nodes we obtain the following identity for the averaged interaction $H_{k,l}$ between k and l:

$$-H_{k,l} = \sum_{j=2}^{N} (E_{m_{kj}}^k \otimes E_{m_{lj}}^l)^\dagger H_{k,l} (E_{m_{kj}}^k \otimes E_{m_{lj}}^l).$$

Since the interactions between all nodes are inverted it follows that H is inverted. □

Similar to the results given in [12] we derive a lower bound for the time overhead for inverting a dynamical evolution as follows.

Lemma 2 (Lower bound on inverting) *Let r be the greatest eigenvalue and q the smallest eigenvalue of the J-matrix representing H. Then $\mu \geq \frac{r}{-q}$ is a lower bound on the overhead for simulating $-H$ by H.*

Proof: Denote the smallest eigenvalue of a matrix A by $\lambda_{\min}(A)$. Then we have

$$-r = \lambda_{\min}(-J) = \lambda_{\min}\Big(\sum_j \tau_j U_j J U_j^T\Big) \geq \tau \lambda_{\min}(J) = \tau q\,.$$

The inequality is due to $\lambda_{\min}(A+B) \geq \lambda_{\min}(A) + \lambda_{\min}(B)$ for the sum of two Hermitian matrices A and B (see [3], Theorem III.2). Since q is negative (J is traceless) we have $\tau \geq -r/q$. □

Consider a fully coupled quantum network, where each pair-interaction is of the form $\sigma_\alpha \otimes \sigma_\alpha$. Then the greatest and smallest eigenvalues of J are $n - 1$ and -1. Lemma 2 gives $n - 1$ as lower bound on the time overhead for inversion.

3 Harmonic oscillators with bilinear couplings

We consider a quantum network, where the n nodes are harmonic oscillators, i. e., their energy values are given by $E = 0, 1, 2, \ldots$. Here we restrict our attention to the case

of energy values less than d and obtain as an approximation a d-dimensional Hilbert space for each oscillator. The Hamiltonian of the uncoupled system is given by

$$H_0 := \sum_{k=1}^{n} h_k \,, \tag{9}$$

where each h_k is the diagonal matrix $\mathrm{diag}(0, 1, \ldots, d-1)$ on the node k. Assume in addition that there is a coupling H_C between the individual harmonic oscillators having the form

$$H_C := \sum_{k,l} c_{kl} a_k a_l^\dagger \tag{10}$$

Here $C = (c_{kl})$ is a real symmetric $n \times n$-matrix with zeros on the diagonal determining the couplings and a_k and $a_l^\dagger$ are the *annihilation* and *creation* operators on the k^{th} and l^{th} oscillator, respectively. The annihilation operator a is defined by

$$a|0\rangle = 0 \,, \qquad a|E\rangle = \sqrt{E}|E-1\rangle \,, \quad E = 1, 2, \ldots, d-1 \,, \tag{11}$$

where $\{|E\rangle \mid E = 0, 1, \ldots, d-1\}$ is an eigenvector basis of the free Hamiltonian of an harmonic oscillator.

Interactions of the form (10) often appear if higher order terms in creation and annihilation operators are neglected and only that part of the total interaction term is considered which commutes with the uncoupled evolution corresponding to H_0.

3.1 Decoupling with difference schemes

The decoupling schemes presented in Section 2 can be used to decouple general pair-interaction Hamiltonians. In this section we consider a specific interaction which allows a more efficient decoupling method using the combinatorial concept of difference matrices (cf. [2, Section VIII]).

The coupling H_C between the harmonic oscillators can be removed by transformations of the form $\exp(ih_k t)$ with $t \in \mathbb{R}$. If the time evolution according to H_C is conjugated by transformations $\exp(ih_k t)$ and $\exp(ih_l s)$ on oscillator k and l, respectively, one part of the coupling term between k and l is multiplied with the factor $\exp(i(s-t))$ and the adjoint part with $\exp(i(t-s))$ since

$$\exp(ih_k t)\exp(ih_l s)\, a_k a_l^\dagger \left(\exp(-ih_k t)\exp(-ih_l s)\right) = \exp(i(s-t))\, a_k a_l^\dagger \,, \tag{12}$$

and a similar expression holds for the adjoint term.

We now characterize $n \times N$ matrices M having complex numbers of modulus one as entries which are suitable for decoupling H_C. Such a matrix M defines a sequence of operations on the n oscillators as follows. If $(e^{it_1}, e^{it_2}, \ldots, e^{it_n})$ denotes the j^{th} column, this means that during the j^{th} time interval the natural time evolution of the n oscillators is conjugated by the local transformation

$$\prod_{k=1}^{n} \exp(ih_k t_k) \,. \tag{13}$$

The total effect of this scheme is that the term $a_k a_l^\dagger$ obtains the factor $\langle m_l | m_k \rangle$, where m_k is the k^{th} row of M and $\langle \cdot | \cdot \rangle$ is the usual inner product in $\mathbb{C}^N$. This gives the following *decoupling criterion*: all couplings are removed if and only if the rows are orthogonal in the usual sense. There is a canonical way of finding n vectors having this property by taking the Fourier transform of the standard basis of $\mathbb{C}^n$. However, the rotations $\exp(2\pi i h_j/n)$ required to be implemented are very close to the identity for large n.

An alternative way of constructing such a matrix is given by difference schemes [2, 9]. We choose the numbers t_k in each row to be of the form $2\pi r/u$ where $u \geq 2$ is a natural number and r is an element of the cyclic group $Z_u = \{0, 1, \ldots, u-1\}$ of order u.

Definition 4 *An $n \times N$ array $D(n, N)$ with entries in Z_u is called a difference scheme based on Z_u if the difference vector of any two rows has the property that each element of Z_u occurs equally often.*

Let $D(n, N)$ be a difference scheme based on Z_u. We construct an $n \times N$ complex matrix M from D by replacing each entry r by $e^{2\pi i r/u}$. The rows of M are vectors in $\mathbb{C}^N$ and since D is a difference scheme they are orthogonal, i. e.,

$$M M^\dagger = N \, \mathbf{1}_N \,. \tag{14}$$

Therefore, M satisfies the decoupling criterion. In view of (14), a difference scheme $D(n, N)$ in which $n = N$ is also called a generalized Hadamard matrix [2, Section VIII] of order n over Z_u. In particularly, any (ordinary) Hadamard matrix of order n is a difference scheme $D(n, n)$ over Z_2.

3.2 Recoupling disjoint cliques

The scheme presented above does not only allow to remove all interactions but also to achieve the following selective recoupling without time overhead. Partition the set of nodes into n' disjoint subsets (called "cliques") and remove only the couplings between nodes in different cliques. This can be achieved by applying the same sequences of transformations on all nodes in the same clique, since this does not affect the interactions among them. Then it is sufficient to construct a difference scheme with only n' rows since each row refers to one of the cliques. Note that an analogous way of "clique decoupling" is also possible for the following kind of n-qubit interaction. Assume that all qubits are coupled by the interaction $\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y + \sigma_z \otimes \sigma_z$. Then the interacting is invariant with respect to simultaneous unitary rotations on both qubits. Hence decoupling schemes for n' qubits define a "clique decoupling" scheme for n' cliques.

3.3 Simulation of different coupling strengths

An interesting problem arises if we want to switch off interactions between arbitrary pairs or, even more general, to weaken the interaction between some of the oscillators. These goals are special instances of the general problem to simulate a coupling Hamiltonian $H_{\tilde{C}}$ using H_C where $\tilde{C}$ is an arbitrary real symmetric coupling matrix.

Now we define a matrix T in such a way that the entry-wise product (Schur-product) of T and C is $\tilde{C}$. Of course this is not possible if an entry of C is equal to zero and the corresponding entry of $\tilde{C}$ does not vanish. This corresponds to the fact that one cannot simulate a coupling between nodes which are not coupled. We choose the vectors m_k introduced in Subsection 3.1 with complex numbers of modulus one such that the corresponding Gram matrix $G = (\langle m_k | m_l \rangle)_{k,l=1,\ldots,n}$ coincides with T on all off-diagonal entries. Note that the diagonal entries of G always give the number of time steps of the simulation. One can generalize this by choosing time steps of different length and define the vectors m_k as mappings from the interval $[0, t]$ to the complex numbers of modulus one. By taking the inner product

$$\langle m_k | m_l \rangle := \int_0^t m_k(t') \overline{m}_l(t') dt'$$

we obtain the same statement as above: the time overhead t is determined by the diagonal entries of G. Note that in our formulation a weak interaction can be used to simulate a strong one since we allow time overhead for the simulation.

A *lower* bound for this overhead is given by the absolute value of the least eigenvalue of T since G being a Gram matrix is positive. This coincides with the eigenvalue criterions stated in [27] derived for n spin 1/2 systems. The lower bound for simulating its own inverse has been shown to be $n-1$ for the spin-spin interaction of the form $\sigma_z \otimes \sigma_z$ [27, 12]. In strong analogy, we obtain the same bound $n-1$ for simulating $-H_C = H_{-C}$ by H_C when C has vanishing terms only on the diagonal, since in this case the corresponding matrix T has only entries -1 except for the diagonal entries which are zero. This proves the bound since the absolute value of the least eigenvalue of T is $n-1$. Note that lower bounds based on the T-matrix do only refer to simulations using unitary transformations of the form $\exp(ih_j t)$ with $t \in \mathbb{R}$. The following theorem shows that the lower bound $n-1$ for time reversal is even valid if *general unitary transformations* on each oscillator and presents an inversion scheme attaining this bound.

Theorem 5 (Optimal inversion) *A time optimal scheme for inverting a coupling of the form H_C as in equation (10) is given by the vectors*

$$m_k := (e^{2\pi i k/n}, e^{2\pi i 2k/n}, \ldots, e^{2\pi i (n-1)/n}).$$

Proof: First note that due to the length of the vectors this simulation has time overhead $n-1$. In order to prove that this is optimal, define the following linearly independent elements of $su(d)$.

$$X_r := |r\rangle\langle r-1| + |r-1\rangle\langle r|$$

and

$$Y_r := i|r\rangle\langle r-1| - i|r-1\rangle\langle r|$$

for $r = 1, \ldots, d-1$. These matrices are orthonormal with respect to the inner product $\langle V|W\rangle := \mathrm{tr}(VW)/2$. One may supplement these $2d-2$ vectors to a orthonormal

basis of $su(d)$, but the completion is irrelevant since the interaction among each pair of oscillators can be written as an expression in X_r and Y_r.

$$a \otimes a^\dagger + a^\dagger \otimes a = \sum_{rs} \sqrt{rs}(X_r \otimes X_s + Y_r \otimes Y_s)\,.$$

The coupling matrix J (see eq. (6)) can be constructed as follows. Define a $(2d-2) \times (2d-2)$-matrix A by

$$A := |\phi\rangle\langle\phi| + |\psi\rangle\langle\psi|\,,$$

with

$$|\phi\rangle := (\sqrt{1}, \sqrt{2}, \ldots, \sqrt{d-1}, 0, \ldots, 0)^T$$

and

$$|\psi\rangle := (0, \ldots, 0, \sqrt{1}, \sqrt{2}, \ldots, \sqrt{d-1})^T\,.$$

With respect to the basis described above, for all pairs (k,l) of oscillators the coupling matrices $J_{k,l}$ are the same and given by completing A by embedding into a $(d^2-1) \times (d^2-1)$-matrix A'. Since the vectors $|\phi\rangle$ and $|\psi\rangle$ are orthogonal, the spectrum of $J_{k,l}$ is $a, a, 0, \ldots, 0$, where $a = \langle\phi|\phi\rangle = \langle\psi|\psi\rangle > 0$. The spectrum of J contains two copies of the value $(n-1)a$ and $n-1$ times the value $-a$. The other eigenvalues are zero. This can be seen by writing J as a tensor product $M \otimes A'$ where M is an $n \times n$-matrix with entries 0 on the diagonal and 1 elsewhere. The smallest value $\tau > 0$ such that the spectrum of τJ majorizes $-J$ is $n-1$. This proves optimality of the time reversal scheme. □

An *upper* bound for the general simulation problem can also be derived in strong analogy to [27] and is given by the so-called *weighted chromatic index* W_T of the matrix T. This concept has been introduced in [11] in a related context in order to quantify the complexity of a general pair-interaction Hamiltonian on n qubits. For each $s \geq 0$ define a graph G_s on the n nodes as vertices which has an edge (k,l) if and only if the absolute value of the entry T_{kl} is greater than s. Let n_s be the chromatic number of G_s (see [4]), i. e., the number of colors required for coloring the edges of G_s in such a way that no two edges with a common node receive the same color. Then define W_T as

$$W_T := \int_0^\infty n_s ds\,,$$

which defines a generalization of the chromatic index for weighted graphs. The key idea to prove this upper bound can easily be understood if one assumes T to have entries of modulus one or zero. Then W_T is the chromatic index of a graph indicating which couplings should not be removed. Given an admissible coloring of this graph, we define a simulation with W_T steps as follows. Each color c defines a step in which we remove all those interactions which are not colored by c. This step can be executed without time overhead as explained in Subsection 3.2. Hence in each step, only the couplings between disjoint oscillator pairs remain.

4 Comparison with other methods

In this section we relate the decoupling method based on orthogonal arrays which was presented in Section 2 to the approach of [17] for the case of decoupling in qubit networks (see also [24] for decoupling in qubit networks based on orthogonal arrays).

Accordingly, let the system Hamiltonian be written in the form

$$H = \sum_{kl;\alpha\beta} J_{kl;\alpha\beta}\sigma_\alpha^k\sigma_\beta^l + \sum_{k;\alpha} r_{k;\alpha}\sigma_\alpha^k\,, \tag{15}$$

where σ_α are the Pauli matrices.

We explain briefly the approach of [17] to construct decoupling schemes. In each interval, each σ_α^k acquires a $+$ or $-$ sign, which is controlled by the applied local unitaries to be described. The coupling $J_{kl;\alpha\beta}\sigma_\alpha^k\sigma_\beta^l$ for $k \neq l$ is unchanged (negated) if the signs of σ_α^k and σ_β^l agree (disagree). Note that the signs of the three Pauli matrices σ_α^k acting on the same qubit k are not independent.

Conjugating with the transformations $\mathbf{1}^k, \sigma_x^k, \sigma_y^k, \sigma_x^l$ the acquired signs for $\sigma_x^k, \sigma_y^k, \sigma_z^k$ are given by $(+++), (+--), (-+-), (--+)$.

Following [17] a decoupling scheme for n qubits that concatenates N intervals can be specified by three $n \times N$ sign matrices S_x, S_y, S_z, related by the entry-wise product $S_x * S_y = S_z$. We say that the three matrices satisfy the Schur condition since this entry-wise product is usually called the Schur product. The (k, j) entry of S_α is the sign of σ_α^k in the j^{th} time interval. Therefore decoupling is achieved if any two rows taken from S_x, S_y, S_z are orthogonal.

The following theorem establishes a connection between decoupling schemes constructed using orthogonal arrays as described in Section 2 and the decoupling schemes specified by sign matrices S_x, S_y, S_z.

Theorem 6 *A decoupling scheme constructed using an orthogonal array $OA(n, N)$ over the alphabet $\mathcal{A} = \{1, 2, 3, 4\}$ and the Pauli basis $\mathcal{E} = \{\mathbf{1}, \sigma_x, \sigma_y, \sigma_z\}$ for all nodes gives rise to sign matrices S_x, S_y, S_z satisfying the Schur and orthogonality conditions.*

Proof: We identify the operators of $\mathcal{E}$ with the elements of $\mathcal{A}$ according to $1 \mapsto \mathbf{1}$, $2 \mapsto \sigma_x$, $3 \mapsto \sigma_y$, and $4 \mapsto \sigma_z$. Conjugating with the operators of $\mathcal{E}$ the Pauli matrices acquire the following signs:

	1	2	3	4
σ_x	$+$	$+$	$-$	$-$
σ_y	$+$	$-$	$+$	$-$
σ_z	$+$	$-$	$-$	$+$

(16)

Starting from the given orthogonal array we now construct the three sign matrices S_x, S_y, and S_z. Pick any two rows k and l of the OA. We may assume that the two rows have the following form (or else we apply a suitable permutation of the columns)

$$\underbrace{\left(\begin{array}{cccc|cccc|cccc|cccc|c} 1&1&1&1&2&2&2&2&3&3&3&3&4&4&4&4&\cdots \\ 1&2&3&4&1&2&3&4&1&2&3&4&1&2&3&4&\cdots \end{array}\right)}_{\lambda \text{ times}} \tag{17}$$

since all pairs appear equally often (λ times) in the OA. Let $\vec{\lambda} = (+ + \cdots +)$ be the vector of length $\lambda = N/16$ containing only $+$. By substituting the entries of the rows k and the l of the OA by the corresponding sign assignments in Table (16) we define the following six rows of S_x, S_y, S_z, respectively:

$$\begin{aligned} S_{x;k} &:= \vec{\lambda} \otimes (++--) \otimes (++++) \\ S_{y;k} &:= \vec{\lambda} \otimes (+-+-) \otimes (++++) \\ S_{z;k} &:= \vec{\lambda} \otimes (+--+) \otimes (++++) \end{aligned}$$

$$\begin{aligned} S_{x;l} &:= \vec{\lambda} \otimes (++++) \otimes (++--) \\ S_{y;l} &:= \vec{\lambda} \otimes (++++) \otimes (+-+-) \\ S_{z;l} &:= \vec{\lambda} \otimes (++++) \otimes (+--+) \,. \end{aligned}$$

Obviously, S_x, S_y, and S_z are orthogonal and satisfy the Schur condition $S_x * S_y = S_z$. □

Finally, we give an alternative proof for the existence of a decoupling scheme for $n = (2^{2m} - 1)/3$ qubits using $N = 2^{2m}$ time intervals. A decoupling scheme with these parameters can be constructed using orthogonal arrays [24] and Hadamard matrices [17].

Let V be the vector space $\mathbb{F}_4^m$, where $m \geq 1$ and let $\mathbb{F}_4 = \{0, 1, \omega, \omega^2 = 1+\omega\}$, where $\omega^3 = 1$, be the Galois field with 4 elements. Recall that the number of d-dimensional subspaces of an m-dimensional vector space over $\mathbb{F}_q$ is given by

$$\left[\begin{array}{c} m \\ d \end{array} \right]_q := \frac{(q^m - 1)(q^{m-1} - 1) \cdots (q^{m-d+1} - 1)}{(q^d - 1)(q^{d-1} - 1) \cdots (q - 1)} \tag{18}$$

(cf. [2, Lemma 2.14, Section I]). For the special case $q = 4$ and $d = 1$ formula (18) shows that there are $(4^m - 1)/(4 - 1) = (2^{2m} - 1)/3$ lines in $\mathbb{F}_4^m$. Note that different lines intersect in the point $\{0\}$ only. Hence by taking the set of all one-dimensional subspaces of $\mathbb{F}_4^m$ we obtain a maximal spread in $\mathbb{F}_4^m$, i. e. a collection of subspaces U_i partitioning $\mathbb{F}_4^m$ with the additional property that

$$U_i \cap U_j = \{0\} \,.$$

We define a map φ from $\mathbb{F}_4$ onto $\{-1, +1\}^4$ as follows:

$$\begin{aligned} \varphi(0) &= (+1, +1, +1, +1) \\ \varphi(\omega) &= (+1, -1, +1, -1) \\ \varphi(\omega^2) &= (+1, +1, -1, -1) \\ \varphi(1) &= (+1, -1, -1, +1) \end{aligned}$$

This is the Hadamard matrix $H_4 = H_2 \otimes H_2$ where H_2 is the usual Hadamard matrix of size 2. Therefore all rows are orthogonal.[5] Note that the last three rows satisfy the Schur condition.

[5]The fact that this matrix is indeed the Hadamard matrix can also be derived with the help of group characters. More precisely, we consider $\mathbb{F}_4$ as a two-dimensional vector space over $\mathbb{F}_2$ and let tr denote the trace map of this field extension [10, Section 4.15]. For all $z \in \mathbb{F}_4$ the map $\varphi(z) : x \mapsto (-1)^{\mathrm{tr}(zx)}$ is an irreducible character of the additive group $(\mathbb{F}_4, +)$ (which is isomorphic to $Z_2 \times Z_2$). Hence, orthogonality of the rows follows from the orthogonality of the characters.

We extend the map φ to vectors $\vec{v} = (v_1, \ldots, v_m) \in \mathbb{F}_4^m$ by defining the map

$$\phi(\vec{v}) := \varphi(v_1) \otimes \cdots \otimes \varphi(v_m) \in \{-1, 1\}^{4m} . \tag{19}$$

The image of ϕ is the set of all rows of the Hadamard matrix $H_2^{\otimes 2m}$. Let $U_k = \langle \vec{v}_k \rangle$ be a maximal spread of $\mathbb{F}_4^m$. By evaluating ϕ on the three elements of U_k (except for the zero vector $\vec{0}$) we get three orthogonal vectors satisfying the Schur condition. We can take them as rows of S_x, S_y, S_z:

$$\begin{aligned} S_{x;k} &= \phi(\omega \cdot \vec{v}_k) \\ S_{y;k} &= \phi(\omega^2 \cdot \vec{v}_k) \\ S_{z;k} &= \phi(1 \cdot \vec{v}_k) \end{aligned}$$

This shows that the second through the last rows of the Hadamard matrix $H_2^{\otimes 2m}$ can be divided into $(2^{2m} - 1)/3$ disjoint 3-subsets, each with rows that satisfy the Schur condition. The rows in a 3-subset can be chosen as rows of S_x,S_y and S_z, respectively.

5 Conclusions

We have shown that pair-interactions between the subsystems of a multipartite quantum system can be decoupled efficiently if a sufficiently large set of local control operations on the subsystems is available. Such decoupling schemes can be constructed using *orthogonal arrays* (a concept of combinatorics). The rows of these arrays define pulse sequences of local operations taken from a *unitary error basis*. We discuss the connection between the decoupling method based on orthogonal arrays and those introduced in [17].

We have shown that mutual simulation of pair-interaction Hamiltonians in multi node systems is possible provided that a so-called *transformer group* of transformations is available.[6] The upper bound $O(n^2)$ on the simulation time is a consequence of the existence of selective decoupling schemes. The construction of a time-optimal simulation leads to a non-trivial convex optimization problem. We have derived a lower bound on the time overhead in terms of the spectrum of the matrix describing the coupling parameters. For some interactions simpler decoupling schemes can be devised: for bilinear coupling of harmonic oscillators selective decoupling can be achieved using so-called *difference schemes*. The condition for time optimality of mutual simulation of different bilinear couplings can concisely be expressed in terms of linear algebra. Based on this we have constructed time optimal schemes for time reversal.

From the results shown in this paper it follows that the time optimal implementation of unitary transformations turns out not to be a matter of optimal factorization into parallelized bilocal quantum gates alone. The transformation has rather to be written as the solution of a time-dependent Schrödinger equation where the occurring Hamiltonians are those which can be simulated with small time overhead. This leads to another definition of *quantum complexity* different from the discrete one measured by counting the number of elementary gates.

[6] Note that similar results have been developed in [20], independently.

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