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UNIVERSAL SIMULATION OF HAMILTONIANS USING A FINITE SET OF CONTROL OPERATIONS

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Any quantum system with a non-trivial Hamiltonian is able to simulate any other Hamiltonian evolution provided that a sufficiently large group of unitary control operations is available. We show that there exist finite groups with this property and present a sufficient condition in terms of group characters. We give examples of such groups in dimension 2 and 3. Furthermore, we show that it is possible to simulate an arbitrary bipartite interaction by a given one using such groups acting locally on the subsystems.

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1. Introduction

Simulating Hamiltonian evolutions of arbitrary quantum systems is an interesting application for future quantum computers. Historically, the idea of simulating Hamiltonian time evolutions was the first motivation for quantum computation [1]. Whereas in early works on this problem the desired Hamiltonian was proposed to be simulated by a discrete sequence of gate operations (see e. g. [2]), a more control theoretic formulation of the problem has become popular recently [3, 4, 5, 6, 7, 8]. In this formulation one assumes that the dynamics of the quantum computer is determined by its Hamiltonian together with external control possibilities. Here the task is to simulate an evolution that would have occurred under some other Hamiltonian by interspersing the natural time evolution with control operations. More explicitly, one assumes that the natural evolution $\exp(-iHt)$ alternates with fast implementations of unitary operations V_j, i. e., the resulting evolution is given by

$$\exp(-iH\tau_N t)V_N \cdots \exp(-iH\tau_2 t)V_2 \exp(-iH\tau_1 t)V_1\,, \tag{1}$$

where the relative times between the control operations are given by τ_i for $i = 1, \ldots, N$. If t is small compared to the time scale of the evolution $\exp(-iHt)$, the resulting evolution is approximatively given by

$$\exp(-i\bar{H}t)\,.$$

Here $\bar{H}$ is the *average Hamiltonian*

$$\bar{H} := \sum_{i=1}^{N} \tau_i U_i^\dagger H U_i \,,$$

where we set $U_i := \prod_{j=1}^{i} V_j$. Important characteristics of simulation schemes like (1) are the amount of operations performed (complexity) and the total operation time (overhead). The average Hamiltonian method is the basis for simulating Hamiltonians by a given one and has applications which go beyond the usual aims of quantum computation. As examples we mention the following applications:

1. **Decoupling / Suppression of Decoherence**

   The time evolution on the joint Hilbert space of a system and its environment can be interspersed with transformations on the system's space alone in such a way that the net effect is a separate ("decoupled") time evolution of the system and the bath [9]. This is a generalization of decoupling techniques in Nuclear Magnetic Resonance [10].

2. **Time inversion**

   The natural time evolution $t \mapsto \exp(-iHt)$ with $t \geq 0$ can be conjugated by unitary transformations in such a way that the total effect is a transformation of the form $\exp(-iHs)$ with negative s. Remarkably, there are schemes for inverting *unknown* Hamiltonians. This fact is closely related to the existence of decoupling schemes [9]. Time inversion for unknown Hamiltonians is a useful primitive in *quantum process tomography*, i. e., procedures that distinguish between unknown time evolutions [11]. The essential idea is that time inversion enables to implement transformations of the form $\exp([H, A])$ for arbitrary self-adjoint A even if H is unknown.

3. **Generating arbitrary time evolutions with a finite control group**

   Assume that the only external control operations of a quantum system are implementations of unitary operations taken from a finite group S. If the natural time evolution is non-trivial and S in a sense is large enough, than every unitary transformation can be generated by concatenations of the natural evolution and elements of S. In particular, this is possible if the natural Hamiltonian H can be transformed into any other in the sense of the average Hamiltonian method.

   This is a special instance of the following problem: Given an arbitrary $\mathbb{R}$-linear map L on the set of self-adjoint traceless operators, the task is to find a sequence of unitary operations such that the system evolves according to the Hamiltonian $L(H)$ if its natural (unknown) Hamiltonian H is present. The problems of inverting or switching off unknown Hamiltonians are special cases of this problem with $L = 0$ or $L(H) = -H$. In its full generality, procedures for simulating $L(H)$ if an unknown H is present can be used as primitives in quantum process tomography [11] and quantum control procedures [12].

4. **Simulating interactions by other ones**

   Consider a bipartite system with Hilbert space $\mathbb{C}^d \otimes \mathbb{C}^d$. Assume that the interaction between both parts is a fixed Hamiltonian on the joint Hilbert space which cannot be controlled at all. The only possibilities to control the system are implementations of local transformations on each of the subsystems. These transformations can be used to imitate other interactions [6, 8].

   In n-partite systems $(\mathbb{C}^d)^{\otimes n}$, where the interaction between each pair of subsystems is assumed to be fixed, one can simulate other pair-interactions in the sense of the average Hamiltonian method. Time optimization of these simulations leads to interesting problems of parallel execution. For n-qubit networks, this problem has been addressed in [5, 13, 7, 14].

The paper is organized as follows. In Section 2 we define what it means to simulate a Hamiltonian and explain the physical meaning in the context of average Hamiltonian theory [10, 15, 16].

In Section 3 we introduce the concept of an *annihilator* for d-dimensional quantum systems characterizing control procedures that switch off the possibly unknown dynamics of the system. These procedures directly give decoupling and inversion schemes. Explicitly, they can be constructed using nice error bases [17, 18] which yield minimal annihilator procedures attaining the lower bound d^2 on the complexity. We show a lower bound on the *overhead* of inversion procedures of a general, possibly unknown Hamiltonian to be $d-1$ and an upper bound of d^2-1. Furthermore, a lower bound on the complexity is shown to be d^2-1.

In Section 4 we address the question how to simulate an arbitrary Hamiltonian by any other if only a restricted set of control operations is available. The condition on the set of available control operations for making universal simulation possible is stronger than the requirement to make annihilation possible. A sufficient condition for a group of available control operations allowing universal simulation can be formulated in terms of group characters. Groups satisfying this criterion will be called *transformer groups*. We present transformer groups for dimensions 2 and 3. Furthermore, we show in Section 5 that the transformer groups allow to transform any interaction in a bipartite system into any other by operating on the subsystems only.

2. Dynamical control

For the implementation of a quantum computer it is necessary to control the time evolution of the used physical system in a universal way. In many physical systems the only directly accessible control possibilities are given by a set of control unitaries and the system Hamiltonian that cannot be switched off. By applying the control operations we effectively change the Hamiltonian into a piecewise constant time-dependent Hamiltonian. The formalism of average Hamiltonian theory [10, 15, 16] allows to solve for the resulting time evolution at a time t by writing the evolution of a time independent average Hamiltonian $\bar{H}$. Following [10, 15, 16] we briefly sketch average Hamiltonian theory: the overall dynamic after a period of evolution is given by

$$U(t) = \mathcal{T} \exp(-i \int_0^t \mathrm{d}\tau H(\tau)) = \exp(-i\bar{H}t)\,,$$

where $\mathcal{T}$ denotes the Dyson time ordering operator. A solution of this equation is a time independent Hamiltonian that would result in the same unitary if it were applied over the same period. If the Hamiltonian $H(\tau)$ commutes with itself at all times we have $\bar{H} = \int_0^t \mathrm{d}\tau \mathrm{H}(\tau)$. However, this is rarely the case. For sufficiently small t, the Magnus expansion provides a formal means of calculating the average Hamiltonian:

$$\bar{H} = \bar{H}^{(0)} + \bar{H}^{(1)} + \bar{H}^{(2)} + \dots \tag{2}$$

where the operators $\bar{H}^{(0)}, \bar{H}^{(1)}, \dots$ are the average Hamiltonians of increasing order

$$\bar{H}^{(0)} = \frac{1}{t}\int_0^t \mathrm{d}\tau \mathrm{H}(\tau), \tag{3}$$

$$\bar{H}^{(1)} = \frac{-i}{2t}\int_0^t \mathrm{d}\tau' \int_0^{\mathrm{t}} \mathrm{d}\tau''[\mathrm{H}(\tau'), \mathrm{H}(\tau'')]\,. \tag{4}$$

We have $\|H^{(0)}\| \leq 1$ and $\|\bar{H}^{(1)}\| \leq t/2$ since $\|[H(\tau'), H(\tau'')]\| \leq 2\|H(\tau')\|\|H(\tau'')\| = 2$ and we are integrating over the simplex of area $t^2/2$. The norm of the higher order terms is bounded by higher orders of t. Therefore for sufficiently small time t the resulting unitary $U(t)$ is essentially determined by $\bar{H}^{(0)}$ (see e.g. [19]).

We assume that the only directly accessible control possibilities are the unitaries in the *control* set $\mathcal{C} \subseteq SU(d)$ and assume in addition that they can be performed arbitrarily fast compared to the natural time evolution. This socalled *fast control limit* is justified e. g. in NMR because the coupled and local evolutions act on significantly different time scales. We will now subject the system to a cyclic pulse train. The pulses are assumed to be infinitely short. A sequence consisting of N pulses will be denoted by

$$P := (V_1, \tau_1, \dots, V_N, \tau_N) \tag{5}$$

where $V_i \in \mathcal{C}$ and $\tau_i > 0$ are relative times, i. e. $\tau_i > 0$ and $\sum_{i=1}^N \tau_i = 1$. The pulses are applied from left to right. If we apply the sequence over the time t the resulting unitary is given by

$$U_P(t) = \prod_{i=1}^{N} \exp(-iH\tau_i t)V_i\,. \tag{6}$$

The τ_i specify the fraction of time between the pulses. For a cyclic sequence (defined by $\prod_{i=1}^N V_i = \mathbf{1}$) we can express the resulting unitary as

$$U_P(t) = \prod_{i=1}^{N} U_i^\dagger \exp(-iH\tau_i t)U_i\,, \tag{7}$$

where $U_i = \prod_{j=1}^i V_j$. Using the identity $U^\dagger \exp(H)U = \exp(U^\dagger H U)$ we get

$$U_P(t) = \prod_{i=1}^{N} \exp(-iH_i\tau_i t)\,, \tag{8}$$

where $H_i = U_i^\dagger H U_i$. These operators are the Hamiltonians in the so-called "toggling frame". Let $Ad_{\mathcal{C}}(H)$ denote set of conjugates of H, i. e.,

$$Ad_{\mathcal{C}}(H) = \{ Ad_U(H) = U^\dagger H U \mid U \in \mathcal{C} \}. \tag{9}$$

Then the unitary $U_P(t)$ is the solution of a time-dependent Schrödinger equation with piecewise constant Hamiltonians in $Ad_{\mathcal{C}}(H)$.

The previous discussion motivates the following definition of the notion of simulating a Hamiltonian by another Hamiltonian.

Definition 1 (First order simulation) *Let $\tilde{H}$ be any Hamiltonian. We say $\tilde{H}$ can be simulated by H with overhead 1, written $\tilde{H} \prec H$, if and only if there are $\tau_i > 0$ summing up to 1 and $H_i \in Ad_{\mathcal{C}}(H)$ such that $\tilde{H} = \sum_j \tau_i H_i$, i. e. $\tilde{H}$ can be written as a convex combination of conjugates of H by elements of $\mathcal{C}$. $\tilde{H}$ can be simulated by H with overhead τ iff $\tilde{H} \prec \tau H$.*

Using this definition of simulation the problem of time-optimal simulation of a Hamiltonian is reduced to a convex optimization problem (this has been noted in [6, 5]).

3. Annihilators

In this section we introduce the concept of an annihilator for a d-dimensional quantum system characterizing control procedures for switching off the possibly unknown dynamics of the system. These procedures directly give decoupling and inversion schemes. We prove some optimality properties of annihilators and show how a minimal annihilator can be explicitly constructed using nice error basis.

Definition 2 (Annihilator) *Let $P := (V_1, \tau_1, V_2, \tau_2, \ldots, V_N, \tau_N)$ be a cyclic pulse sequence of length N, i. e. $\tau_i > 0$, $\sum_{i=1}^N \tau_i = 1$, and $\prod_{i=1}^N V_i = \mathbf{1}$. Set $U_i = \prod_{j=1}^i V_j$. The sequence P is called an annihilator of dimension d and length N iff*

$$\sum_{i=1}^N \tau_i U_i^\dagger a U_i = 0 \tag{10}$$

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

Theorem 1 (Minimal annihilator) *A minimal annihilator has length d^2. Furthermore all relative times τ_i of a minimal annihilator are equal.*

Proof: Let $(V_1, \tau_1, V_2, \tau_2, \ldots, V_N, \tau_N)$ be an arbitrary annihilator. The corresponding $U_i = \prod_{j=1}^i V_j$ and τ_i define a realization of the depolarizing channel Λ on $\mathbb{C}^d$ by random external fields [20] since

$$\Lambda(\rho) = \sum_{i=1}^N \tau_i U_i^\dagger \rho U_i = \mathbf{1}/d. \tag{11}$$

This permits to show that $N \geq d^2$ as follows: by sending one part of a maximally entangled state $|\Psi\rangle\langle\Psi|$ in $\mathbb{C}^d \otimes \mathbb{C}^d$ through the depolarizing channel we end up with the maximally mixed state $\mathbf{1}/d^2$. Therefore we need at least d^2 unitaries since the rank of each $(\mathbf{1} \otimes U_i^\dagger)|\Psi\rangle\langle\Psi|(\mathbf{1} \otimes U_i)$ is 1 and they must sum up to d^2 (the rank of the maximally mixed state). For $N = d^2$ all τ_i

must be equal for entropy reasons (see [21], page 518) since for $\tau_i \neq \frac{1}{d^2}$

$$S\left(\sum_{i=1}^{d^2} \tau_i (\mathbf{1} \otimes U_i^\dagger)|\Psi\rangle\langle\Psi|(\mathbf{1} \otimes U_i)\right) \leq H(\tau_1, \tau_2, \ldots, \tau_{d^2}) < \log_2 d^2 = S(\mathbf{1}/d^2)\,,$$

where S denotes the von Neumann and H the Shannon entropy. The existence of a minimal annihilator is guaranteed due to the concept of nice error basis to be introduced in the next subsection. □

Theorem 1 shows that a minimal annihilator corresponds to a unitary error depolarizer [22] and thus to a unitary basis. The connection between annihilators and unitary error basis has already been mentioned in [23].

3.1. *Nice error bases*

In this section we deal with the problem to construct a minimal annihilator. For this we construct bases for the vector-space $\mathbb{C}^{d\times d}$ of $d \times d$-matrices which consist entirely of unitary matrices and are orthogonal with respect to the trace inner product. One way of constructing such bases relies on the concept of *nice error bases*. We refer to [17] and [18] for an overview of this method and mention that nice error bases are used in the construction of quantum error control codes [24, 25, 26, 27]. They are also of interest in the theory of noiseless subsystems [28, 29] and in connection with the development of quantum authentication codes [30].

Definition 3 *Let G be a group of order d^2 with identity element e. A* nice error basis *on $\mathbb{C}^d$ is a set $\mathcal{E} = \{U_g \in \mathcal{U}(d) \mid g \in G\}$ of unitary matrices such that*

(i) U_e *is the identity matrix,*

(ii) $\operatorname{tr} U_g = d\,\delta_{g,e}$ *for all* $g \in G$,

(iii) $U_g U_h = \alpha(g,h) U_{gh}$ *for all* $g, h \in G$,

where the factor system $\alpha(g,h)$ is a function from $G \times G$ to the set $\mathbb{C}^\times := \mathbb{C} \setminus \{0\}$.

In [18] it was shown that the map $g \mapsto U_g$ defines a projective representation of G; this is a consequence of conditions (i) and (iii). Condition (ii) shows that the matrices U_g are pairwise orthogonal with respect to the trace inner product $\langle A, B\rangle := \operatorname{tr}(A^\dagger B)/d$. Hence, a nice error basis is an irreducible projective representation of the finite group G. The group G itself is also called *index group* since its group elements index the elements of the nice error basis $\mathcal{E}$.

Note that in general the group generated by the matrices U_g for $g \in G$ will be larger than G, since these matrices are not closed under multiplication. A well-known theorem from projective representation theory (cf. [31, Theorem V.24.6], [32, Theorem 11.15]) states that it is always possible to switch to an equivalent projective representation such that the images U_g generate a finite group $\hat{G}$ (see also [18]). This group is called the *abstract error group* corresponding to $\mathcal{E}$. Whereas $g \mapsto U_g$ is an irreducible projective representation of G, this yields an irreducible *ordinary* representation of $\hat{G}$. It is a well-known fact that $\hat{G}$ is a central extension of G (cf. [32]): denoting the center of $\hat{G}$ by $\zeta(\hat{G})$ this means that $\hat{G}/\zeta(\hat{G}) \cong G$.

Given a nice error basis $\{U_g \mid g \in G\}$, then the abstract error group is isomorphic to the group generated by the matrices U_g. The assumption that the factor system α is of finite order ensures that the abstract error group is finite.

Example 1 (Heisenberg group) The discrete Fourier transform of length $d \in \mathbb{N}$ is the unitary transformation defined by $\mathrm{DFT}_d := \frac{1}{\sqrt{d}}(\omega^{k\cdot l})_{k,l=0,\ldots,d-1}$, where ω denotes the primitive d-th root of unity $e^{2\pi i/d}$. Define $\mathcal{E}_d := \{S^i T^j : i = 0,\ldots,d-1, j = 0,\ldots,d-1\}$, where

$$S := \begin{pmatrix} 0 & 1 & & & \\ & \ddots & \ddots & & \\ & & \ddots & 1 & \\ & & & 0 & \\ 1 & & & & \end{pmatrix}, \quad T := \mathrm{DFT}_d^{-1} \cdot S \cdot \mathrm{DFT}_d = \begin{pmatrix} 1 & & & & \\ & \omega & & & \\ & & \ddots & & \\ & & & \omega^{d-1} & \end{pmatrix}.$$

Here again ω is the primitive d-th root of unity $e^{2\pi i/d}$. Then $\mathcal{E}_d$ is a nice error basis on $\mathbb{C}^d$ showing the existence of nice error bases for any dimension $d \in \mathbb{N}$ of the underlying system. The index group in this case is the abelian group $G = Z_d \times Z_d$ whereas the corresponding abstract error group is a nonabelian group isomorphic to a semi-direct product $\hat{G} \cong (Z_d \times Z_d) \rtimes Z_d$ (the so-called Heisenberg group). The projective representation of G leading to the error basis $\mathcal{E}_d$ is defined by mapping the generators of G as follows: $(1,0) \mapsto S$ and $(0,1) \mapsto T$. The identity $ST = \omega TS$ is readily verified which shows that the commutator subgroup of $\hat{G}$ is contained in the center $\zeta(\hat{G})$. This also shows that the factor system α corresponding to the projective representation of G defined $\mathcal{E}_d$ is given by

$$\alpha((i,j),(k,l)) = \omega^{-jk},$$

for all $(i,j),(k,l) \in G$.

We give a brief account of some general properties of nice error bases (see also [18]). A complete classification of abstract error groups on $\mathbb{C}^d$ for $1 \leq d \leq 11$ was given in [18]. Index groups of abstract error groups are in general not abelian: in [18] a family of groups having nonabelian index groups was constructed. It is known that all abstract error groups are solvable. Moreover, it is known that all solvable groups can occur as *subgroups* of index groups of nice error bases. On the other hand, it is known that not all solvable groups can occur as index groups.

3.2. *Averaging and Annihilation*

Using the concept of abstract error groups we describe the idea of switching off an interaction by averaging over a group. Whereas usual techniques are based on ordinary irreducible representations [9, 23], the following lemma shows that averaging over a projective irreducible representation also projects onto the set of scalar matrices.

Lemma 1 *Let $M \in \mathbb{C}^{d\times d}$, G be a finite group, and $R : g \mapsto U_g \in \mathcal{U}(d)$ an irreducible projective representation of G. Then the following equation holds:*

$$\frac{1}{|G|}\sum_{g\in G} U_g^\dagger M U_g = \frac{\mathrm{tr}(M)}{d}\,\mathbf{1}$$

Proof: We have seen that each projective representation of an index group G with associated factor system α gives rise to an ordinary representation of the corresponding abstract error group $\hat{G}$ and that $\hat{G}$ is a central extension of G. It follows that $\{U_g : g \in G\}$ is a set of coset

representatives for $\zeta(\hat{G})$ in $\hat{G}$, i. e.,

$$\hat{G} = \bigcup_{g \in G} \zeta(\hat{G}) U_g.$$

Each element $\sigma \in \hat{G}$ has a unique factorization of the form $\sigma = zg$ where $z \in \zeta(\hat{G})$ and $g \in G$. From Schur's Lemma (cf. [33, Section 2.2]) follows that for $M \in \mathbb{C}^{d \times d}$, $\hat{G}$ a finite group, and $R : \sigma \mapsto U_\sigma \in \mathcal{U}(d)$ an irreducible (ordinary) representation of $\hat{G}$ the following identity holds:

$$\frac{1}{|\hat{G}|} \sum_{\sigma \in \hat{G}} U_\sigma^\dagger M U_\sigma = \frac{\mathrm{tr(M)}}{d} \mathbf{1}. \tag{12}$$

Using this we obtain

$$\begin{aligned} \frac{1}{|G|} \sum_{g \in G} U_g^\dagger M U_g &= \frac{1}{|G|} \frac{1}{|\zeta(\hat{G})|} \sum_{g \in G} \sum_{z \in \zeta(\hat{G})} U_g^\dagger U_z^\dagger M U_z U_g \\ &= \frac{1}{|\hat{G}|} \sum_{\sigma \in \hat{G}} U_\sigma^\dagger M U_\sigma \\ &= \frac{\mathrm{tr}(M)}{d} \mathbf{1}, \end{aligned}$$

where the last line is due to Schur's Lemma (12) for ordinary representations. □

3.3. *Decoupling*

We consider a bipartite quantum system (e. g. a system coupled to a bath) living on the joint Hilbert space $\mathcal{H}_S \otimes \mathcal{H}_B$. Here $\mathcal{H}_S$ and $\mathcal{H}_B$ denote the Hilbert spaces of S and B respectively. Let $su(\mathcal{H})$ denote the Lie algebra of traceless self-adjoint matrices acting on the Hilbert space $\mathcal{H}$. The Hamiltonian can be written as

$$H = H_S \otimes \mathbf{1}_B + \mathbf{1}_S \otimes H_B + H_{SB}\,, \tag{13}$$

where $H_S \in su(\mathcal{H}_S)$ is the free system Hamiltonian, $H_B \in su(\mathcal{H}_B)$ is the free bath Hamiltonian, and H_{SB} describes the coupling between the system and the bath, i. e. $H_{SB} = \sum_j A_j \otimes B_j$ with $A_j \in su(\mathcal{H}_S)$ and $B_j \in su(\mathcal{H}_B)$. In order to protect the evolution of S against the effect of the interaction H_{SB} we seek a cyclic pulse sequence as a suitable decoupling interaction.

By applying the pulse sequence of an annihilator we get

$$\tilde{H} = \frac{1}{|G|} \sum_{g \in G} (U_g^\dagger \otimes \mathbf{1}) H (U_g \otimes \mathbf{1}) = \mathbf{1}_S \otimes H_B\,. \tag{14}$$

This shows that decoupling can be achieved using an annihilator procedure on only one of the subsystems (cf. [23, 9]).

3.4. *Inversion of Hamiltonians*

We consider the problem to invert an arbitrary, possibly unknown Hamiltonian, i. e. to simulate $-H$ given the Hamiltonian H.

We can use the following trick [11]: by averaging over all elements of G but the identity we can invert the Hamiltonian

$$\sum_{g\in G\setminus\{1\}} U_g^\dagger H U_g = -H \tag{15}$$

because of Lemma 1 (note that H is traceless). The resulting time overhead is $|G|-1 = d^2-1$ and the complexity is d^2-1. This can be seen as a generalization of the refocussing technique used in NMR (see e.g. [34, 35]). In general, the inverted time evolution will be slower than the original one:

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

Proof: Write $-H$ as a positive linear combination of conjugates of H as in Definition 1. Let $\lambda_{\min}(A)$ be the smallest eigenvalue of an operator A. Then we have

$$-r = \lambda_{\min}(-H) = \lambda_{\min}\Big(\sum_i \tau_i U_i^\dagger H U_i\Big) \geq \tau\lambda_{\min}(H) = \tau q.$$

The inequality is due to $\lambda_{\min}(A+B) \geq \lambda_{\min}(A) + \lambda_{\min}(B)$ (see [36], Theorem III.2) for the sum of two Hermitian matrices A and B. Since q is negative it follows that $-r/q \leq \tau$. □

For the Hamiltonian $H = \mathrm{diag}(\mathrm{d}-1, -1, \ldots, -1)$ the overhead is at least $d-1$. Therefore a lower bound on time overhead for inverting an unknown Hamiltonian is $d-1$.

4. Universal transformation of Hamiltonians

In Section 3 we have given a necessary and sufficient condition on the minimal set of available control operations in order to enable inversion and cancelling of Hamiltonians. If we want to simulate an arbitrary Hamiltonian by any other this condition is not sufficient. This can be seen by the following example. Assume that the only control operations on $\mathbb{C}^2$ are given by the Pauli-matrices (in their role as unitary operators). If the Hamiltonian $H := \sigma_z$ is given, conjugation of H by a Pauli-matrix can only lead to either H or $-H$. All the Hamiltonians which can be obtained as average Hamiltonians are scalar multiples of H. Hence one cannot simulate e. g. σ_x. The following concept will be useful in order to find groups which enable universal simulation.

Definition 4 (Transformer) *A subgroup $\mathcal{T}$ of $SU(d)$ is called a universal transformer of Hamiltonians iff every $\mathbb{R}$-linear map L on $su(d)$ (i. e., the set of self-adjoint traceless operators) can be written as*

$$L(A) = \sum_j p_j U_j^\dagger A U_j$$

with positive real numbers p_j and $U_j \in \mathcal{T}$.

The physical of this is that a transformer allows to simulate the Hamiltonian $L(H)$ if the *unknown* Hamiltonian H is present. In [11] it has been shown that $SU(d)$ is a transformer for every dimension d.

Observation 1 *In particular, a transformer is able to simulate an arbitrary Hamiltonian $\tilde{H} \in su(d)$ by an arbitrary Hamiltonian $H \in su(d)$.*

Remarkably, the condition for a finite group to be a transformer can be characterized in terms of irreducibility of certain representations. In contrast to the condition for an annihilator, it refers to the adjoint action on the set of operators instead of the underlying Hilbert space.

Definition 5 (Adjoint action) *Let G be a finite group and φ a unitary representation of degree d, i. e., φ operates on $V = \mathbb{C}^d$. We define a linear representation φ_{ad} on $V \otimes V$ by $\varphi_{\mathrm{ad}}(g) := \overline{\varphi(g)} \otimes \varphi(g)$ for all $g \in G$, where $\overline{U}$ denotes complex conjugation of a matrix U. We call φ_{ad} the* adjoint action *of φ. Note that this action can be identified with the action of G on matrices via conjugation $g \mapsto (M \mapsto \varphi(g)^\dagger M \varphi(g))$.*

In the following we make use of the fact that the algebra generated by the images of an irreducible m-dimensional representation ϑ of a finite group G over the complex numbers is equal to the full matrix algebra $\mathbb{C}^{m\times m}$. We cite the corresponding theorem from [32, Theorem 9.2]. Recall that a representation ϑ defined over a field F is called *absolutely irreducible* if it remains irreducible when considered over an extension field E/F.

Theorem 2 *Let ϑ be an absolutely irreducible representation of a finite group G which has degree m and is defined over the field F. Then*

$$\Big\{ \sum_{g\in G} \alpha_g \vartheta(g) : \alpha_g \in F \Big\} = F^{m\times m}.$$

In particular for any m-dimensional irreducible representation over the field $\mathbb{C}$ of complex numbers the vector space generated by the images equals $\mathbb{C}^{m\times m}$.

We now have the necessary prerequisites to characterize finite transformers.

Theorem 3 (Characterization of finite transformers)
A finite group $\mathcal{T} \leq SU(d)$ is a transformer if and only if the adjoint representation ϑ given by

$$\vartheta(U) := (A \mapsto U^\dagger A U)$$

with $U \in \mathcal{T}$ acts irreducibly on $sl(d) = su(d) + i\, su(d)$, i. e., the space of traceless operators.

Proof: ($\Leftarrow$) Let L be a given $\mathbb{R}$-linear map on $su(d)$ and assume that the adjoint action of $\mathcal{T}$ is irreducible on $sl(d)$ and denote this representation by ϑ. From Theorem 2 follows that the complex linear span of the images of ϑ is the full matrix algebra acting on $sl(d)$. Hence, the mapping L can be written as a complex linear combination of the form $L : A \mapsto \sum_i q_i U_i^\dagger A U_i$. We now show that the coefficients can be chosen to be real: since $U_i^\dagger A U_i$ is self-adjoint for all i we have $L(A) = L(A)^\dagger = \sum_i \overline{q_i} U_i^\dagger A U_i$. Therefore we can write L in the form $L : A \mapsto \sum_i p_i U_i^\dagger A U_i$ with coefficients $p_i = \frac{1}{2}(q_i + \overline{q}_i) \in \mathbb{R}$. Using the inversion scheme of Section 3.4 we can chose the coefficients p_i to be positive real numbers.

($\Rightarrow$) Assume that every $\mathbb{R}$-linear map on $su(d)$ can be implemented in the sense of Definition 4 using $\mathcal{T}$. Let $\mathcal{M}$ be the complex linear span of the maps $\vartheta(U)$ with $U \in \mathcal{T}$. The idea is

to show that any $F \in sl(d)$, $F \neq 0$ can be mapped to any other $\tilde{F} \in sl(d)$ by a map $T \in \mathcal{M}$. This in turn shows that the adjoint action is irreducible since there cannot be a nontrivial invariant subspace. To construct T proceed as follows. Let $F = H_1 + iH_2$ with $H_1, H_2 \in su(d)$. Assume w.l.o.g. that $H_1 \neq 0$, otherwise multiply F by $-i$. The set $\mathcal{M}$ contains maps L_1 and L_2 with $L_1(H_1) = \tilde{H}_1$, $L_1(H_2) = \lambda\tilde{H}_1$ and $L_2(H_1) = \tilde{H}_2$, $L_2(H_2) = \mu\tilde{H}_2$ with $\mu, \lambda \in \mathbb{R}$. Then $T := L_1/(1+\lambda) + i\,L_2/(1+\mu)$ is the desired map. □

4.1. *Finite transformers*

We derive a necessary and sufficient condition for a finite group to be a transformer group in the sense of Definition 4. Theorem 3 shows that the problem to construct a finite transformer group is to find for given dimension $d > 1$ a finite group G and an irreducible (unitary) representation φ of G such that the adjoint action becomes irreducible if we split off the trivial representation $\mathbf{1}$ of G. The trivial representation is always contained in φ_{ad} since the one-dimensional space corresponding to the linear span of the identity matrix remains invariant, i. e., $\varphi_{\mathrm{ad}} = \mathbf{1} \oplus \pi$ for some representation π of G. Abusing the notation we will write $\varphi_{\mathrm{ad}} - \mathbf{1}$ to denote the summand π in this decomposition.

Once we have found a suitable pair (G, φ) with $\deg(\varphi) = d$ this yields a transformer group as in Definition 4. For basic results concerning representation theory of finite groups we refer the reader to [32].

Example 2 *We examine the case of a two-dimensional system, i. e., $d = 2$. Starting from the Pauli matrices*

$$\sigma_x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma_y := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \sigma_z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

we first note that the group $\langle i\cdot\sigma_x, i\cdot\sigma_y, i\cdot\sigma_z\rangle$ is isomorphic to the quaternion group Q_8 of order 8. This group has an (outer) automorphism of order 3 which permutes the Pauli matrices cyclically. This automorphism is given by the matrix

$$R := \frac{i-1}{2}\begin{pmatrix} i & i \\ -1 & 1 \end{pmatrix}.$$

Setting $s_k := i\sigma_k$ for $k \in \{x, y, z\}$ the automorphism is given by $R^{-1}s_xR = s_y$, $R^{-1}s_yR = s_z$, and $R^{-1}s_zR = s_x$. The group generated by the s_k and R is isomorphic to $\mathrm{SL}(2, \mathbb{F}_3)$, i. e., the group of 2×2 matrices over the finite field $\mathbb{F}_3$ which have determinant 1. Let φ be the (natural) representation of the matrix group given by $\langle s_x, s_y, s_z, R\rangle$. Then the 24 matrices in the image of φ form a faithful irreducible representation of $\mathrm{SL}(2, \mathbb{F}_3)$. Choosing the basis $\{s_x, s_y, s_z\}$ of $sl(2)$ we see that the images of $\varphi_{\mathrm{ad}} - \mathbf{1}$ are given explicitly by $s_x \mapsto \mathrm{diag}(1, -1-1)$, $s_y \mapsto \mathrm{diag}(-1, 1, -1)$, $s_z \mapsto \mathrm{diag}(-1, -1, 1)$, and R maps to the permutation matrix corresponding to the 3-cycle $(1, 2, 3)$. It is readily verified that this is an irreducible representation.

Let G be a finite group having an irreducible representation φ such that the images of φ are a transformer in the sense of Definition 4. Then necessarily φ must be nonmonomial* for otherwise the set of diagonal matrices would be an invariant subspace under the action of $\varphi_{\mathrm{ad}} - \mathbf{1}$. Note that in fact the group $\mathrm{SL}(2, \mathbb{F}_3)$ is the smallest group which is not an $\mathcal{M}$-group,

*A representation is called *monomial* if all representing matrices have the property to contain precisely one non-vanishing entry in each row and each column.

i. e., $\mathrm{SL}(2,\mathbb{F}_3)$ has representations which are not equivalent to monomial ones. Therefore a necessary condition for φ to be a transformer has been found.

There is a necessary and sufficient characterization of transformer groups which can be verified from the character table alone. Recall that the character χ of a representation φ is defined by $\chi(g) := \mathrm{tr}(\varphi(g))$ and that a character is called irreducible iff the corresponding representation is irreducible.

Theorem 4 *Let G be a finite group and χ be an irreducible character of G with corresponding representation φ. Then χ corresponds to a universal transformer if and only if the following identity holds:*

$$\sum_{g\in G} |\chi(g)|^4 = 2|G|.$$

Proof: The representation $\varphi_{\mathrm{ad}} - \mathbf{1}$ has character values $|\chi(g)|^2 - 1$ for all $g \in G$ since $\mathrm{tr}(\varphi_{\mathrm{ad}}(g)) = \overline{\chi(g)}\chi(g)$. Recall that the vector space of class functions on G has a normalized scalar product given by

$$\langle \chi_1 | \chi_2 \rangle = \frac{1}{|G|} \sum_{g\in G} \chi_1(g)\chi_2(g^{-1})$$

for characters χ_1, χ_2 of G. A character χ is irreducible iff $\langle\chi|\chi\rangle = 1$. Computing the latter scalar product of the character corresponding to $\varphi_{\mathrm{ad}} - \mathbf{1}$ we obtain

$$\begin{aligned} \frac{1}{|G|}\sum_{g\in G}(|\chi(g)|^2-1)\cdot(\overline{|\chi(g)|^2-1}) &= \frac{1}{|G|}\sum_{g\in G}|\chi(g)|^4 - \frac{2}{|G|}\sum_{g\in G}|\chi(g)|^2 + 1 \\ &= \frac{1}{|G|}\sum_{g\in G}|\chi(g)|^4 - 1 \end{aligned}$$

On the other hand this scalar product is equal to 1 due to the irreducibility of $\varphi_{\mathrm{ad}} - \mathbf{1}$. Rearranging terms and clearing denominators yields the claimed statement. □

In the following we present a transformer for a three dimensional system. The minimal group having a representation φ for which $\varphi_{\mathrm{ad}} - \mathbf{1}$ is irreducible is the linear group $\mathrm{GL}(3,\mathbb{F}_2)$ of invertible 3×3 matrices over the field $\mathbb{F}_2$. This is a simple group of order 168. As generators of this group we choose the matrices

$$x := \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},\ y := \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix},$$

where x is an element of order 2 and the order of y is 7. The group $\mathrm{GL}(3,\mathbb{F}_2)$ has a three-dimensional irreducible representation φ over the complex numbers which on the generators x and y is given by the following assignments:

$$\varphi(x) := \frac{2}{\sqrt{7}} \begin{pmatrix} \cos(\frac{5\pi}{14}) & -\zeta_7^3\cos(\frac{\pi}{14}) & -\zeta_7^2\cos(\frac{3\pi}{14}) \\ -\zeta_7^4\cos(\frac{\pi}{14}) & -\cos(\frac{3\pi}{14}) & \zeta_7^6\cos(\frac{5\pi}{14}) \\ -\zeta_7^5\cos(\frac{3\pi}{14}) & \zeta_7\cos(\frac{5\pi}{14}) & -\cos(\frac{\pi}{14}) \end{pmatrix},\ \varphi(y) := \begin{pmatrix} \zeta_7 & \cdot & \cdot \\ \cdot & \zeta_7^2 & \cdot \\ \cdot & \cdot & \zeta_7^4 \end{pmatrix}.$$

Table 1. Transformer groups of small sizes

Group size	Numbers in library	Dimension
24	3	2
48	28, 29, 33	2
72	3, 25	2
96	67, 74, 192	2
120	5	2
144	36, 121, 122, 157	2
168	22	2
168	42	3
192	187, 204, 963	2
216	3, 38	2
216	88	3
240	93, 102, 103, 154	2

Here $\cdot$ is an abbreviation for 0 and ζ_7 denotes the primitive 7-th root of unity $e^{2\pi i/7}$. The character of the representation φ takes the values

$$3,\ -1,\ 1,\ 0,\ \zeta_7+\zeta_7^2+\zeta_7^4,\ \zeta_7^3+\zeta_7^5+\zeta_7^6$$

on the conjugacy classes of $\mathrm{GL}(3,\mathbb{F}_2)$. Consulting the character table of $\mathrm{GL}(3,\mathbb{F}_2)$ in the Atlas [37, p. 3] we find that φ is irreducible. The representation $\varphi_{\mathrm{ad}}-\mathbf{1}$ has character values

$$8,\ 0,\ 0,\ -1,\ 1,\ 1$$

from which follows that it is also irreducible, again by checking the character table of $\mathrm{GL}(3,\mathbb{F}_2)$. Overall we obtain that the representation φ of $\mathrm{GL}(3,\mathbb{F}_2)$ yields a transformer of size 168. Using the Neubüser catalogue used in MAGMA and GAP, cf. [38, 39] we performed an exhaustive search over all groups of smaller sizes which has shown that this indeed is the minimal possible group size.

In Tabular 1 we summarize the results of this search. Groups of sizes up to 255 have been considered. The number in the Neubüser catalogue is given such that for instance the first row of this table corresponds to the group (in GAP syntax) `SmallGroup(24,3)` which has been studied in Example 2. Note that we only give transformer groups which act faithfully.

4.2. *Lower bound on the overhead*

In the following we derive a lower bound on the time overhead for simulating a Hamiltonian using an arbitrary transformer. We need some results on majorization and doubly stochastic matrices (cf. [40] for a summary). 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 with equality when $k = d$ [36].

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

$$\mathrm{Spec(A + B)} \prec \mathrm{Spec(A)} + \mathrm{Spec(B)}\,. \tag{16}$$

This permits us to derive a lower bound on the simulation overhead.

Lemma 3 (Lower bound) *A lower bound on the overhead of simulating $\tilde{H}$ by H is given by the minimal τ such that*

$$\mathrm{Spec}(\tilde{\mathrm{H}}) \prec \tau \mathrm{Spec(H)}\,. \tag{17}$$

Proof: This follows from Definition 1 and inequality (16). □

We now consider the question when this lower bound can be attained. Let $H = \sum_{i=1}^{d} \lambda_i |i\rangle\langle i|$ and $\tilde{H} = \sum_{i=1}^{d} \mu_i |i\rangle\langle i|$ where $|i\rangle$ is a basis of eigenvectors. Let τ be minimal such that $\vec{\mu} \prec \tau\vec{\lambda}$. We set $d' := d - 1$. We have $(\mu_1, \ldots, \mu_{d'}) \prec (\tau\lambda_1, \ldots, \tau\lambda_{d'})$ since $\sum_i \mu_i = \sum_i \lambda_i = 0$ (the Hamiltonians are traceless). This is equivalent to the existence of a doubly stochastic matrix D with $D(\lambda_1, \ldots, \lambda_{d-1})^T = (\mu_1, \ldots, \mu_{d-1})^T$. By Birkhoff's theorem we can decompose a doubly stochastic matrix as a convex sum of permutations, i. e.

$$D = \sum_{\sigma \in \Sigma} p_\sigma U_\sigma \tag{18}$$

where U_σ is the permutation matrix associated to σ, i. e. maps the basis vector $|i\rangle$ to $|\sigma(i)\rangle$, and and Σ is a subset of the symmetric group $S_{d'}$. The $d' \times d'$ doubly stochastic matrices form a $({d'}^2 - 2d' + 1)$-dimensional convex set. The extreme points are the permutation matrices. Carathéodory's theorem guarantees that a point in a m-dimensional compact convex set may be expressed as a convex combination of at most $m + 1$ extremal points of that set. Therefore every doubly stochastic matrix can be written as a convex combination of at most ${d'}^2 - 2d' + 2 = (d-2)^2 + 1$ permutations.

We view the matrices U_σ as $d \times d$ matrices that fix the basis vector $|d\rangle$. We have

$$\tilde{H} = \tau \sum_{\sigma \in \Sigma} p_\sigma U_\sigma^\dagger H U_\sigma \tag{19}$$

The lower bound can be attained in particular if the transformer contains the matrices permuting the eigenvectors of H and and the matrix realizing the base change between the eigenvector basis of H and $\tilde{H}$.

Let H be the system Hamiltonian. Let σ be the cyclic shift, i. e. $\sigma(i) = i + 1 \mod d$ and U_σ the corresponding matrix. Than we can switch off the Hamiltonian

$$\sum_{j=0}^{d-1} \frac{1}{d} U_{\sigma^j}^\dagger H U_{\sigma^j} = 0 \tag{20}$$

with complexity at most d provided that we can perform the shift with the transformer. In this case we can also invert it with complexity and overhead at most $d - 1$. However, when the Hamiltonian is not known we need at least d^2 operations to switch it off.

5. Simulation of bipartite Hamiltonians

The following theorem shows that all bipartite Hamiltonians can be simulated by any Hamiltonian (with non-trivial coupling and non-trivial local terms) provided that the set of available unitary transformations contains a transformer for each of the subsystems. Let $B = \{\sigma_\alpha \mid \alpha = 1, \ldots, d^2 - 1\}$ be a basis of $su(d)$.

Theorem 5 *Let an arbitrary interaction*

$$H := \sum_{\alpha\beta} J_{\alpha\beta}\sigma_\alpha \otimes \sigma_\beta + a \otimes \mathbf{1} + \mathbf{1} \otimes b$$

be given with $a, b \in su(d)$ with $a, b \neq 0$. Let $\mathcal{T}_1$ and $\mathcal{T}_2$ be transformers of the left and the right subsystem, respectively. Assume that it is possible to implement all unitary transformations of the form $U \otimes V$ with $U \in \mathcal{T}_1$ and $V \in \mathcal{T}_2$. Then H can be used for simulating any arbitrary $\tilde{H}$ with $\tilde{H} := \sum_{\alpha\beta} \tilde{J}_{\alpha\beta}\sigma_\alpha \otimes \sigma_\beta + \tilde{a} \otimes \mathbf{1} + \mathbf{1} \otimes \tilde{b}$ i. e., there are positive numbers τ_j, $U_j \in \tau_1$ and $V_j \in \tau_2$ such that

$$\tilde{H} = \sum_j \tau_j (U_j^\dagger \otimes V_j^\dagger) H (U_j \otimes V_j)\,. \tag{21}$$

Proof: We first consider the case that the local terms are all zero. Write H in the form

$$H = \sum_j A_j \otimes B_j\,,$$

where A_j and B_j are elements of $su(d)$ and all B_j are linearly independent and all A_j are nonzero. Then H can be transformed into any interaction of the form $C \otimes D$ with arbitrary $C, D \in su(d)$. This can be done by choosing $\mathbb{R}$-linear maps L_1 and L_2 on $su(d)$ with $L_1(A_1) = C$, $L_2(B_1) = D$, and $L_2(B_j) = 0$ for $j \neq 1$. Since $\mathcal{T}_1$ and $\mathcal{T}_2$ are universal transformers one can find positive numbers d_j and f_j and unitary transformations $U_j \in \mathcal{T}_1$ and $V_j \in \mathcal{T}_2$ such that

$$L_1(\cdot) = \sum_j d_j U_j^\dagger \cdot U_j \quad \text{and} \quad L_2(\cdot) = \sum_j f_j V_j^\dagger \cdot V_j\,.$$

Hence we obtain

$$\sum_{ij} d_i f_j (U_i^\dagger \otimes V_j^\dagger) H (U_i \otimes V_j) = C \otimes D\,.$$

This proves that we can simulate each tensor product operator $C \otimes D$. By setting $C := \tilde{J}_{\alpha\beta}\sigma_\alpha$ and $D := \sigma_\beta$ we can simulate each term in eq. (21). Hence it is possible to simulate $\tilde{H}$. Let H contain local terms. Starting from H we can simulate the Hamiltonian

$$H' = \sum_{\alpha\beta} \tilde{J}_{\alpha\beta}\sigma_\alpha \otimes \sigma_\beta + a' \otimes \mathbf{1} + \mathbf{1} \otimes b'\,,$$

that coincides with the desired Hamiltonian $\tilde{H}$ except for the local terms. Starting from H we can simulate the Hamiltonian $(\tilde{a} - a') \otimes \mathbf{1}$ by applying an annihilator on the right and suitable transformations on the left. Finally, we use a similar scheme for $\mathbf{1} \otimes (\tilde{b} - b')$. □

Note that this proof also applies if the dimensions of the two subsystems are different.

6. Conclusions

We have shown that there are finite groups of unitary control operations which allow to simulate an arbitrary Hamiltonian $\tilde{H}$ by another arbitrary H, i. e., a system with Hamiltonian H can be driven to evolve as if its Hamiltonian were $\tilde{H}$. This can be accomplished using fast sequences of control operations interspersing the natural time evolution. We even found finite groups which allow to solve the following more general control problem: for every linear trace preserving map L on the set of self-adjoint operators the system can be made to evolve according to the Hamiltonian $L(H)$ although its true *unknown* Hamiltonian is H. We have called such groups *transformer groups* and showed that a finite group G has this property if and only if its adjoint action on the set of traceless operators is irreducible. We have characterized finite groups G with this property using characters of representations of G on the Hilbert space. This criterion allows to perform an exhaustive search over groups of small order (up to 255). We found transformer groups for two and three dimensional quantum systems. It remains an open problem to construct finite transformer groups for all dimensions. In bipartite systems, every non-trivial interaction can simulate any other provided that transformer groups on each subsystem can be implemented.

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