Efficient Combinatorial Schemes for Decoupling and Simulating Hamiltonians

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Simulation of Hamiltonians

- let $\mathcal{H} := \mathbb{C}^d$ be a closed quantum system with Hamiltonian H
- we want to effectively change H to the desired Hamiltonian $\tilde{H}$
- a simulation scheme adds a time-dependent control Hamiltonian $H_c(t)$
- $H_c(t)$ is chosen such that the resulting dynamics is described by the effective Hamiltonian H_{eff} with

$$H_{\mathrm{eff}} = \tilde{H}$$

Simulation Tasks

- annihilation / maximal decoupling / time suspension

$$H \quad \mapsto \quad \tilde{H} = \mathbf{0}$$

- time-inversion / spin echo / Loschmidt echo

$$H \quad \mapsto \quad \tilde{H} = -H$$

- general simulation

$$H \quad \mapsto \quad \tilde{H}$$

Simulation with Bang-Bang Controls

- the natural time evolution can be interspersed with unitary bang-bang control operations V_j drawn from some finite set $\mathcal{C}$

$$V_N \exp(-iH\tau_N) \cdots V_2 \exp(-iH\tau_2)\, V_1 \exp(-iH\tau_1)$$

- the control scheme is cyclic: $V_N V_{N-1} \cdots V_1 = \mathbf{1}$
- the corresponding control propagators are $U_1 := \mathbf{1}$ and $U_j := V_{j-1} \cdots V_1$ for $j = 1, \ldots, N-1$
- the resulting dynamics can be expressed as

$$U_N^\dagger \exp(-iH\tau_N)U_N \cdots U_2^\dagger \exp(-iH\tau_2)\, U_2 U_1^\dagger \exp(-iH\tau_1)U_1$$

Pictorial Representation

b.b. operations			V_1		V_2			V_{N-1}		V_N
		τ_1		τ_2		$\cdots$			τ_N	
propagators	U_1		U_2		U_3			U_N		U_1

Effective Hamiltonian

- define the cycle length $T_c := \sum_{j=1}^{N} \tau_j$
- define the time points $t_M := MT_c$ for $M \in \mathbb{N}$
- the stroboscopic dynamics $U(t_M)$

$$U(t_M) := \left(U_N^\dagger \exp(-iH\tau_N)U_N \cdots U_1^\dagger \exp(-iH\tau_1)U_1\right)^M$$

can be expressed as

$$U(t_M) = \exp(-i\bar{H}t_M)$$

for a time-independent effective Hamiltonian $\bar{H}$

Effective Hamiltonian

- Magnus expansion $\bar{H} = \bar{H}^{(0)} + \bar{H}^{(1)} + \bar{H}^{(2)} + \ldots$

$$\bar{H}^{(0)} = \frac{1}{T_c} \sum_{j=1}^{N} \tau_j U_j^\dagger H U_j$$

$$\bar{H}^{(1)} = \frac{-i}{2T_c} \sum_{1 \leq j < k \leq N} \tau_j \tau_k [U_j^\dagger H U_j, U_k^\dagger H U_k]$$

- $\|\bar{H}^{(m)}\| / \|\bar{H}^{(0)}\|$ are of order T_c^m for all m
- $\Rightarrow$ truncation yields more and more accurate approximation as the fast control limit $T_c \rightarrow 0$ is approached

Approximation

- we focus on first-order simulation

$$\bar{H}^{(0)} = \frac{1}{T_c} \sum_{j=1}^{N} \tau_j U_j^\dagger H U_j$$

- by symmetrizing the control cycle

$$U_j = U_{N-j} \quad \text{and} \quad \tau_j = \tau_{N-j}$$

  the terms $\bar{H}^{(m)}$ can be made zero for all odd m

- $\Rightarrow$ the simulation error is only $O(T_c^2)$

Summary: Bang-Bang Simulation

- let $\mathcal{C}$ be the set of available bang-bang controls
- assume that the desired Hamiltonian $\tilde{H}$ can be expressed as

$$\tilde{H} = \sum_{j=1}^{N} \tau_j U_j^\dagger H U_j$$

with $V_j = U_j U_{j-1}^\dagger \in \mathcal{C}$

- then we can simulate $\exp(-i\tilde{H})$ with N control operations, cycle time $T_c = \sum_j \tau_j$, and error $O(T_c^2)$

Simulation with Bounded-Strength Controls

- the assumption of bang-bang control is highly unrealistic
- more realistically, assume that the control Hamiltonian satisfies the properties
  - $\|H_c(t)\| \leq B$
  - $H_c(t)$ is a smooth function
- can we still simulate Hamiltonians?

  can we say something about time, number of control operations, and accuracy of the simulation?

Control Propagator

- a simulation scheme is most conveniently constructed by directly looking at the propagator

$$U_c(t) = \mathcal{T} \exp \left\{ -i \int_0^t H_c(\tau) d\tau \right\}$$

- the control scheme is still cyclic

$$U_c(t + T_c) = U_c(t)$$

for some cycle time T_c and all t

Effective Hamiltonian

- the stroboscopic dynamics $U(t_M)$ with $t_M = MT_c$ and $M \in \mathbb{N}$ can be described by

$$U(t_M) = \exp(-i\bar{H}t_M)$$

for a time-independent effective Hamiltonian $\bar{H}$

- Magnus expansion $\bar{H} = \bar{H}^{(0)} + \bar{H}^{(1)} + \bar{H}^{(2)} + \dots$

$$\bar{H}^{(0)} = \frac{1}{T_c}\int_0^{T_c} U_c^\dagger(\tau) H U_c(\tau)\, d\tau$$

Group-Theoretic Tools

- let G be a finite group and $\mathcal{U} := \{U_g \, : \, g \in G\}$ a set of unitary matrices acting on $\mathcal{H} := \mathbb{C}^d$ s.t.

  the map $g \mapsto U_g$ is compatible with multiplication in G up to phase factors: $U_{gh} = \omega(g,h) U_g U_h$ with $|\omega(g,h)| = 1$

- assume that G and $\mathcal{U}$ are chosen s.t.

$$\frac{1}{|G|} \sum_{g \in G} U_g^\dagger X U_g = \frac{\mathrm{Trace}(X)}{d} \mathbf{1}_d$$

  for any operator X acting on $\mathcal{H}$

- let $S \subset G$ be a generating set for G: every element in G can be written as a product of elements in S

Example

- $\mathcal{H} := \mathbb{C}^2$, $G := Z_2 \times Z_2$, and $\mathcal{U} := \{\mathbf{1}, X, Y, Z\}$

$$\begin{aligned} (0,0) &\mapsto \mathbf{1} \\ (1,0) &\mapsto X \\ (0,1) &\mapsto Z \\ (1,1) &\mapsto Y \end{aligned}$$

- generalizes to $\mathcal{H} := \mathbb{C}^d$

Elementary Control Hamiltonians

assume we can physically implement the generators $s \in S$:

we can obtain U_s as control propagators by switching on some suitably chosen bounded-strength time-dependent control Hamiltonians $h_s(t)$ over $[0, \Delta]$

$$U_s = u_s(\Delta)$$

where

$$u_s(\delta) = \mathcal{T}\left\{\exp(-i\int_0^\delta h_s(t)dt\right\}$$

for $\delta \in [0, \Delta]$

Group / Graph - Theoretic Tools

- let $\Gamma := \Gamma(G, S)$ be the Cayley graph of G with respect to the generating set S
  - the vertices are group elements $g \in G$
  - the directed edges are labeled by generators $s \in S$
  - there is an edge from g to h iff

$$gs = h$$

Examples of Cayley Graphs

- $G := Z_2 \times Z_2$ and $S = \{(0,1),(1,0)\}$

$$\begin{array}{ccc} (0,1) & \leftrightarrow & (1,1) \\ \updownarrow & & \updownarrow \\ (0,0) & \leftrightarrow & (1,0) \end{array}$$

- $G := Z_3 \times Z_3$ and $S = \{(0,1),(1,0)\}$

$$\begin{array}{ccccccc} & \uparrow & & \uparrow & & \uparrow & \\ \rightarrow & (0,2) & \rightarrow & (1,2) & \rightarrow & (2,2) & \rightarrow \\ & \uparrow & & \uparrow & & \uparrow & \\ \rightarrow & (0,1) & \rightarrow & (1,1) & \rightarrow & (2,1) & \rightarrow \\ & \uparrow & & \uparrow & & \uparrow & \\ \rightarrow & (0,0) & \rightarrow & (1,0) & \rightarrow & (2,0) & \rightarrow \\ & \uparrow & & \uparrow & & \uparrow & \end{array}$$

Group / Graph - Theoretic Tools

- a sequence $(g_1, s_1; g_2, s_2; \ldots; g_N, s_N)$ of group elements and generators is called an Euler cycle iff
  - $g_{j+1} = g_j s_j$ for $j = 1, \ldots, N-1$
  - $g_N s_N = g_1$
  - each pair (g, s) occurs exactly once in the sequence for all $g \in G$ and $s \in S$

w.l.o.g we choose g_1 to be the identity element e

Properties of Euler Cycles

the Euler cycle

- visits every vertex $g \in G$ exactly $|S|$ times
- each vertex g is left via each of the s-labeled edges ($s \in S$) exactly once

  $\Rightarrow N = |S||G|$

Example

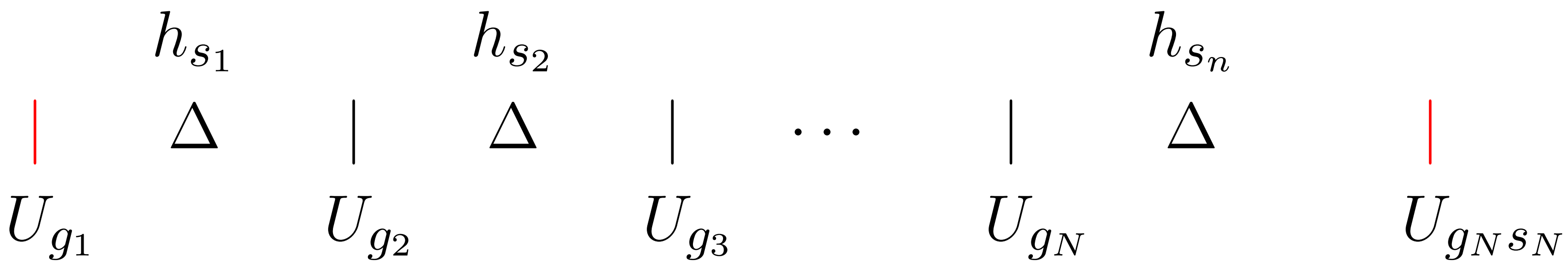
- $G := Z_2 \times Z_2$ and $S = \{(0,1),(1,0)\}$

$$\begin{array}{ccc} (0,1) & \leftrightarrow & (1,1) \\ \updownarrow & & \updownarrow \\ (0,0) & \leftrightarrow & (1,0) \end{array}$$

Euler cycle: start at $(0,0)$, go clockwise, and then go counter-clockwise

Annihilation Based on Euler Cycles

- let $(g_1, s_1; g_2, s_2; \ldots; g_N, s_N)$ be an Euler cycle
- set the cycle length $T_c := N\Delta$
- the control Hamiltonian $H_c(t)$ is obtained by switching on the elementary control Hamiltonians according to the Euler cycle



Analysis of Euler Annihilation Scheme

- to analyze the resulting dynamics it is very useful to define the map Π_G

$$\Pi_G(X) = \frac{1}{|G|} \sum_{g \in G} U_g^\dagger X U_g$$

  and the maps F_s for $s \in S$

$$F_S(X) = \frac{1}{|S|} \sum_{s \in S} \int_0^\Delta \frac{1}{\Delta} u_s(t)^\dagger X u_s(t) dt$$

- Why?

  INTUITION: recall that each pair (g, s) occurs exactly once in the Euler cycle

Analysis of Euler Annihilation Scheme

- the effective Hamiltonian can be expressed as

$$\begin{aligned}\bar{H} &= \frac{1}{T_c}\int_{t=0}^{T_c} U_c(t)^\dagger H U_c(t)dt \\ &= \Pi_G[F_S(H)] \\ &= \mathbf{0}\end{aligned}$$

Euler Simulation Scheme

- assume the desired Hamiltonian can be written as

$$\tilde{H} = \sum_{g \in G} \tau_g U_g^\dagger H U_g$$

- set $T_c := N\Delta + \sum_g \tau_g$
- implement the Euler annihilation cycle, but wait for $\tau_{g_j}/|S|$ after each g_j

	$h_{s_{j-1}}$		$\mathbf{0}$		h_{s_j}		$\mathbf{0}$	
$\vert$	Δ	$\vert$	$\frac{\tau_{g_j}}{\vert S\vert}$	$\vert$	Δ	$\vert$	$\frac{\tau_{g_{j+1}}}{\vert S\vert}$	$\vert$
$U_{g_{j-1}}$		U_{g_j}		U_{g_j}		$U_{g_{j+1}}$		$U_{g_{j+1}}$

Analysis of Euler Simulation Scheme

- the effective Hamiltonian can be expressed as

$$\begin{aligned}\bar{H} &= \frac{1}{T_c}\int_{t=0}^{T_c} U_c(t)^\dagger H U_c(t) dt \\ &= \Pi_G[F_S(H)] + \frac{1}{T_c}\sum_{g\in G} \tau_g U_g^\dagger H U_g \\ &= \frac{1}{N\Delta + \sum_g \tau_g}\,\tilde{H}\end{aligned}$$

the term $N\Delta$ does not occur when b.b. controls are available

Combinatorial Bang-Bang Annihilation

- assume that the quantum system $\mathcal{H} := (\mathbb{C}^2)^{\otimes n}$ consists of n coupled qubits

- assume that the set of bang-bang control operations is $\mathcal{C} := \{\mathbf{1}, X, Y, Z\}^{\otimes n}$, i.e., the qubits can addressed individually

- $\Rightarrow$ the set of control propagators is $\mathcal{U} := \{\mathbf{1}, X, Y, Z\}^{\otimes n}$

Inefficient Annihilation Scheme

- apply the control operations to the qubits in such that each unitary in $\mathcal{U} := \{\mathbf{1}, X, Y, Z\}^{\otimes n}$ is obtained exactly once as control propagator

- this defines an annihilation scheme since

$$\frac{1}{4^n} \sum_{U \in \mathcal{U}} U^\dagger X U = \frac{\mathrm{Trace}(X)}{4^n} \mathbf{1}_{4^n}$$

  for any operator acting on $\mathcal{H} := (\mathbb{C}^2)^{\otimes}$

- this scheme is highly inefficient since the number of control operations is $N = 4^n$ and the cycle time $T_c = 4^n \Delta$

  bad: exponential scaling with the number of qubits n

2-local Hamiltonian

- we take advantage of the fact that the system Hamiltonian is 2-local

$$H := \sum_{k<l} H_{kl}$$

where H_{kl} denotes couplings between qubits k and l

Orthogonal Arrays

- let $\mathcal{A}$ be a finite set of cardinality s and $n, N \in \mathbb{N}$
- an $n \times N$ array A with entries from $\mathcal{A}$ is an orthogonal array with
  - $s = |\mathcal{A}|$ levels
  - strength t
  - index λ

iff every $t \times N$ sub-array of A contains each possible t-tuple of elements in $\mathcal{A}$ precisely λ times as a column

Example

- an orthogonal array with parameters $N = 16$, $n = 5$, $s = 4$, and $t = 2$

$$\begin{pmatrix} \mathbf{1} & \mathbf{1} & \mathbf{1} & \mathbf{1} & X & X & X & X & Y & Y & Y & Y & Z & Z & Z & Z \\ \mathbf{1} & X & Y & Z & Z & Y & X & \mathbf{1} & \mathbf{1} & X & Y & Z & Z & Y & X & \mathbf{1} \\ \mathbf{1} & Y & Z & X & \mathbf{1} & Y & Z & X & Y & \mathbf{1} & X & Z & Y & \mathbf{1} & X & Z \\ \mathbf{1} & Y & Z & X & Z & X & \mathbf{1} & Y & Z & X & \mathbf{1} & Y & \mathbf{1} & Y & Z & X \\ \mathbf{1} & X & Y & Z & X & \mathbf{1} & Z & Y & Z & Y & X & \mathbf{1} & Y & Z & \mathbf{1} & X \end{pmatrix}$$

Construction of OAs

Theorem: Construction of OAs from error-correcting codes

- let C be a linear $[n, k, d]_q$ code over $\mathbb{F}_q$
- let $d^\perp$ be the minimum distance of the dual code $C^\perp$
- arrange the code words of C into the columns of a matrix $M \in \mathbb{F}_q^{n \times q^k}$

  $\Rightarrow M$ is an $OA(q^k, n, q, d^\perp - 1)$

Annihilation Schemes based on OA

- apply the bang-bang control operations on the qubits such that the resulting control propagators follow the columns of the orthogonal array $OA(n, N, 4, \lambda)$
- this defines an annihilation scheme for arbitrary (even unknown) 2-local Hamiltonians on n qubits with N control operations and cycle time $T_c = N\Delta$
- it is efficient since N scales only linearly with n

Combinatorial Euler Annihilation

- assume that the available bounded-strength control Hamiltonians $h_X(t)$ and $h_Z(t)$ implement the unitary operations X and Z if they are switch on for time Δ
- assume that these control Hamiltonians can be realized on the qubits in $\mathcal{H} = (\mathbb{C}^2)^{\otimes n}$ individually

Euler Orthogonal Arrays

- we combined Euler annihilation with orthogonal arrays
- this yields annihilation schemes for arbitrary 2-local Hamiltonians on n qubits with $N = O(n \log n)$ control operations and cycles time $T_c = O(n \log N\Delta)$
- the cost is only increased by the factor $\log n$ compared to the bang-bang setting

Conclusion

- adjust these techniques to realistic scenarios
- extend to open system setting

$$H = H_S \otimes \mathbf{1}_E + \mathbf{1}_S \otimes H_E + \sum_a S_a \otimes B_a$$

  - simulation of Hamiltonians while decoupling from the environment

$$H \quad \mapsto \quad \tilde{H}_S \otimes \mathbf{1}_E + \mathbf{1}_S \otimes H_E$$

  - simulation of open system Hamiltonian

$$H \quad \mapsto \quad \tilde{H}_S \otimes \mathbf{1}_E + \mathbf{1}_S \otimes H_E + \sum_a \tilde{S}_a \otimes B_a$$