Efficient Combinatorial Schemes for Decoupling and Simulating Hamiltonians

Pawel M. Wocjan

School of Electrical Engineering and Computer Science
University of Central Florida
Orlando
wocjan@cs.ucf.edu
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 $H_{\text{eff}}$ with $H_{\text{eff}} = \tilde{H}$.
Simulation Tasks

- annihilation / maximal decoupling / time suspension

\[ H \iff \tilde{H} = 0 \]

- time-inversion / spin echo / Loschmidt echo

\[ H \iff \tilde{H} = -H \]

- general simulation

\[ H \iff \tilde{H} \]
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 $C$

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

- the control scheme is cyclic: $V_N V_{N-1} \cdots V_1 = 1$

- the corresponding control propagators are $U_1 := 1$ 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

\[
\begin{array}{cccccc}
 & V_1 & V_2 & V_{N-1} & V_N \\
\tau_1 & \tau_2 & \cdots & \tau_N \\
\hline
U_1 & U_2 & U_3 & U_N & U_1
\end{array}
\]

propagators
Effective Hamiltonian

- define the cycle length $T_c := \sum_{j=1}^{N} \tau_j$
- define the time points $t_M := M T_c$ 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 $\tilde{H} = \tilde{H}^{(0)} + \tilde{H}^{(1)} + \tilde{H}^{(2)} + \ldots$

\begin{align*}
\tilde{H}^{(0)} &= \frac{1}{T_c} \sum_{j=1}^{N} \tau_j U_j^\dagger H U_j \\
\tilde{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]
\end{align*}

$\| \tilde{H}^{(m)} \| / \| \tilde{H}^{(0)} \|$ are of order $T_c^m$ for all $m$

$\Rightarrow$ truncation yields more and more accurate approximation as the fast control limit $T_c \to 0$ 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 \( m \)

\[ \Rightarrow \text{the simulation error is only } O(T_c^2) \]
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 $\bar{H} = \bar{H}^{(0)} + \bar{H}^{(1)} + \bar{H}^{(2)} + \ldots$

$$\bar{H}^{(0)} = \frac{1}{T_c} \int_0^{T_c} U_c^\dagger(\tau) H U_c(\tau) \, d\tau$$
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: $U_{gh} = \omega(g, h)U_gU_h$ with $|\omega(g, h)| = 1$

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

\[
\frac{1}{|G|} \sum_{g \in G} U_g^\dagger X U_g = \frac{\text{Trace}(X)}{d} 1_d
\]

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

1. \( \mathcal{H} := \mathbb{C}^2, \ G := Z_2 \times Z_2, \text{ and } \mathcal{U} := \{ 1, X, Y, Z \} \)

\[
\begin{align*}
(0, 0) & \mapsto 1 \\
(1, 0) & \mapsto X \\
(0, 1) & \mapsto Z \\
(1, 1) & \mapsto Y
\end{align*}
\]

2. 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 $\delta \in [0, \Delta]$
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

- $G := \mathbb{Z}_2 \times \mathbb{Z}_2$ and $S = \{(0, 1), (1, 0)\}$
  
  \begin{align*}
  (0, 1) & \leftrightarrow (1, 1) \\
  (0, 0) & \leftrightarrow (1, 0)
  \end{align*}

- $G := \mathbb{Z}_3 \times \mathbb{Z}_3$ and $S = \{(0, 1), (1, 0)\}$

\begin{align*}
\uparrow & \quad \uparrow & \quad \uparrow \\
\rightarrow & \quad (0, 2) & \rightarrow (1, 2) & \rightarrow (2, 2) & \rightarrow \\
\uparrow & \quad \uparrow & \quad \uparrow \\
\rightarrow & \quad (0, 1) & \rightarrow (1, 1) & \rightarrow (2, 1) & \rightarrow \\
\uparrow & \quad \uparrow & \quad \uparrow \\
\rightarrow & \quad (0, 0) & \rightarrow (1, 0) & \rightarrow (2, 0) & \rightarrow \\
\uparrow & \quad \uparrow & \quad \uparrow 
\end{align*}
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
  \[ g_{j+1} = g_j s_j \quad \text{for} \quad j = 1, \ldots, N - 1 \]
  \[ g_N s_N = g_1 \]
  - 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

\[ G := \mathbb{Z}_2 \times \mathbb{Z}_2 \text{ and } S = \{(0, 1), (1, 0)\} \]

(0, 1) ↔ (1, 1)

(0, 0) ↔ (1, 0)

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

\[
\begin{align*}
&h_{s_1} & &h_{s_2} & &h_{s_n} \\
&U_{g_1} & &U_{g_2} & &U_{g_3} & &\cdots & &U_{g_N} & &U_{g_N s_N} \\
&\Delta & &\Delta & &\Delta & &\Delta &
\end{align*}
\]
Analysis of Euler Annihilation Scheme

- to analyze the resulting dynamics it is very useful to define the map $\Pi_G$

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

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
the effective Hamiltonian can be expressed as

\[
\bar{H} = \frac{1}{T_c} \int_{t=0}^{T_c} U_c(t)\, H U_c(t) dt
\]

\[
= \Pi_G[F_S(H)]
\]

\[
= 0
\]
Euler Simulation Scheme

- assume the desired Hamiltonian can be written as

\[
\hat{H} = \sum_{g \in G} \tau_g U_g^\dagger H U_g
\]

- set \( T_c := N \Delta + \sum_g \tau_g \)

- implement the Euler annihilation cycle, but wait for \( \tau_{g_j}/|S| \) after each \( g_j \)

\[
\begin{array}{cccccc}
h_{s_{j-1}} & 0 & h_{s_j} & 0 \\
\tau_{g_j}/|S| & \Delta & \tau_{g_j+1}/|S| & \Delta \\
U_{g_{j-1}} & U_{g_j} & U_{g_j} & U_{g_{j+1}} \\
\end{array}
\]
the effective Hamiltonian can be expressed as

\[ \tilde{H} = \frac{1}{T_c} \int_{t=0}^{T_c} U_c(t)\dagger H U_c(t) dt \]

\[ = \Pi_G[F_S(H)] + \frac{1}{T_c} \sum_{g \in G} \tau_g U_g\dagger H U_g \]

\[ = \frac{1}{N\Delta + \sum g \tau_g} \tilde{H} \]

the term \( N\Delta \) does not occur when b.b. controls are available
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 $\mathcal{C} := \{1, X, Y, Z\} \otimes n$, i.e., the qubits can be addressed individually

$\Rightarrow$ the set of control propagators is $\mathcal{U} := \{1, X, Y, Z\} \otimes n$
Inefficient Annihilation Scheme

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

- this defines an annihilation scheme since

\[
\frac{1}{4^n} \sum_{U \in \mathcal{U}} U^\dagger X U = \frac{\text{Trace}(X)}{4^n} 1_{4^n}
\]

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 $\lambda$

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

An orthogonal array with parameters $N = 16$, $n = 5$, $s = 4$, and $t = 2$
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 $\Delta$

- assume that these control Hamiltonians can be realized on the qubits in $\mathcal{H} = (\mathbb{C}^2)^\otimes n$ individually
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

\[ H = H_S \otimes 1_E + 1_S \otimes H_E + \sum_a S_a \otimes B_a \]

- simulation of Hamiltonians while decoupling from the environment

\[ H \rightarrow \tilde{H}_S \otimes 1_E + 1_S \otimes H_E \]

- simulation of open system Hamiltonian

\[ H \rightarrow \tilde{H}_S \otimes 1_E + 1_S \otimes H_E + \sum_a \tilde{S}_a \otimes B_a \]