Techniques for preparing eigenstates of fermionic Hamiltonians

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September 11, 2019

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Overview

- Antisymmetrizing the wavefunction

  [Berry et al., Improved Techniques for Preparing Eigenstates of Fermionic Hamiltonians, NPJ QI 2018]

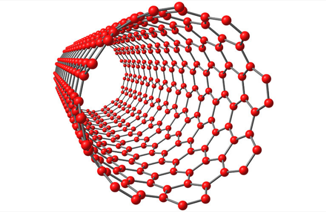
- Simulating time-dependent Hamiltonians

  [Kieferová et al., Simulating the dynamics of time-dependent Hamiltonians with a truncated Dyson series, PRA 2019]

our recent review:

[Cao et al., Quantum Chemistry in the Age of Quantum Computing, Chem. Rev. 2019]

Quantum Computing for Chemistry and Material Science

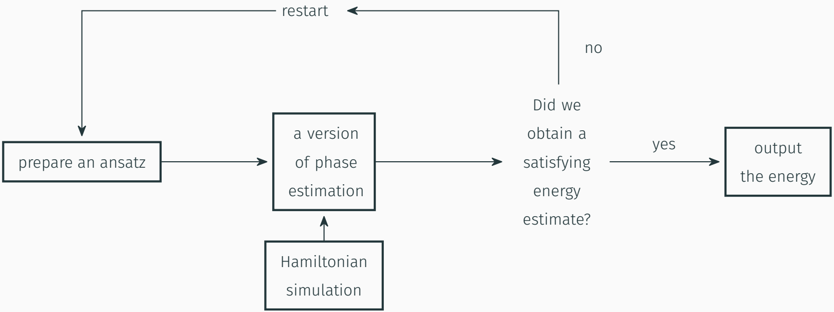


Algorithms for fault-tolerant quantum computers - beyond NISQ.

[credit: PharmaFactz, 123RF.com, Safety+Health Magazine]

Eigenenergy Estimation

Goal: compute the ground state energy of a molecule



[Abrams, Lloyd PRL (1997), Aspuru-Guzik et al. Science (2005)]

Antisymmetrization

First Quantization

State of m electrons, N sites/orbitals.

Fermions in the 1st quantization - symmetry is captured by the state.

- classically intractable
- typically better scaling than 2nd quantization for quantum algorithms

Preparation of Fermionic States

Input: ordered list of occupied orbitals

Output: completely antisymmetric state

$$|r_1 \cdots r_m\rangle \mapsto \sum_{\sigma \in S_m} (-1)^{\pi(\sigma)} \left|\sigma\left(r_1, \cdots, r_m\right)\right\rangle$$

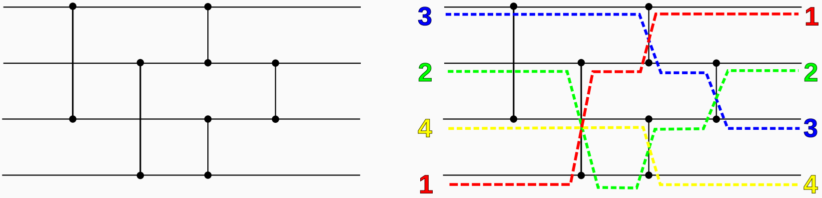
where $\pi(\sigma)$ is the parity of the permutation σ, and $r_p < r_{p+1}$.

NEW: Two approaches based on a classical (Fisher-Yates) shuffle and on reversed sort.

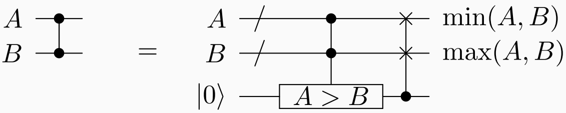
[Abrams, Lloyd PRL (1997)]

Sorting Network

Data-oblivious and reversible sort



[Batcher 1968, Knuth 1968, source:wikipedia]

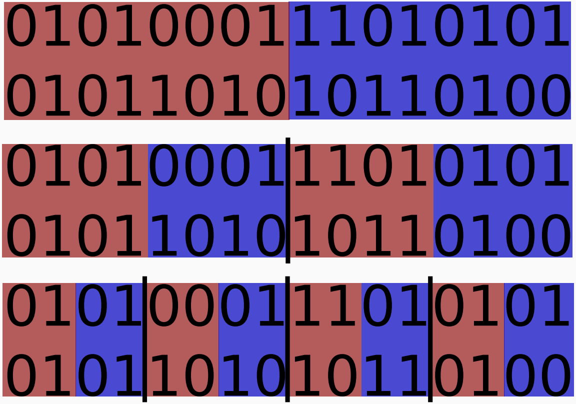


Bitonic sort requires $\mathcal{O}(m \log^2 m)$ comparators.

Coherent Comparison - Divide and Conquer

01010001 11010101
01011010 10110100

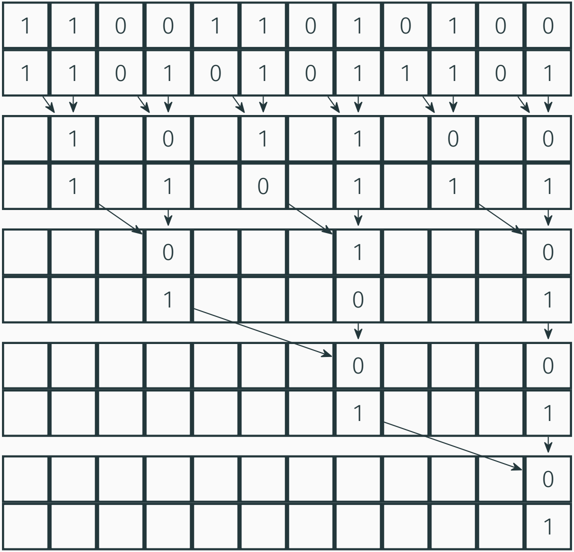
Compare each part separately and then merge the outcomes for the final comparison.



Only ever compare pairs of bits.

Gate count $\mathcal{O}(\log N)$, depth $\mathcal{O}(\log \log N)$.

How Does the Comparison work?



Reverse the algorithm to uncompute

	→	$\|0\rangle\|0\rangle$	→	$\|0\rangle\|0\rangle\|\text{no swap}\rangle$	→	~~$\|0\rangle\|0\rangle\|\text{no swap}\rangle$~~
	→	$\|0\rangle\|1\rangle$	→	$\|0\rangle\|1\rangle\|\text{no swap}\rangle$	→	$\|0\rangle\|1\rangle\|\text{no swap}\rangle$
	→	$\|0\rangle\|2\rangle$	→	$\|0\rangle\|2\rangle\|\text{no swap}\rangle$	→	$\|0\rangle\|2\rangle\|\text{no swap}\rangle$
	→	$\|0\rangle\|3\rangle$	→	$\|0\rangle\|3\rangle\|\text{no swap}\rangle$	→	$\|0\rangle\|3\rangle\|\text{no swap}\rangle$
	→	$\|1\rangle\|0\rangle$	→	$\|0\rangle\|1\rangle\|\text{swap}\rangle$	→	$\|0\rangle\|1\rangle\|\text{swap}\rangle$
	→	$\|1\rangle\|1\rangle$	→	$\|1\rangle\|1\rangle\|\text{no swap}\rangle$	→	~~$\|1\rangle\|1\rangle\|\text{no swap}\rangle$~~
	→	$\|1\rangle\|2\rangle$	→	$\|1\rangle\|2\rangle\|\text{no swap}\rangle$	→	$\|1\rangle\|2\rangle\|\text{no swap}\rangle$
	→	$\|1\rangle\|3\rangle$	→	$\|1\rangle\|3\rangle\|\text{no swap}\rangle$	→	$\|1\rangle\|3\rangle\|\text{no swap}\rangle$
$\|0\rangle\|0\rangle$	→	$\|2\rangle\|0\rangle$	→	$\|0\rangle\|2\rangle\|\text{swap}\rangle$	→	$\|0\rangle\|2\rangle\|\text{swap}\rangle$
	→	$\|2\rangle\|1\rangle$	→	$\|1\rangle\|2\rangle\|\text{swap}\rangle$	→	$\|1\rangle\|2\rangle\|\text{swap}\rangle$
	→	$\|2\rangle\|2\rangle$	→	$\|2\rangle\|2\rangle\|\text{no swap}\rangle$	→	~~$\|2\rangle\|2\rangle\|\text{no swap}\rangle$~~
	→	$\|2\rangle\|3\rangle$	→	$\|2\rangle\|3\rangle\|\text{no swap}\rangle$	→	$\|2\rangle\|3\rangle\|\text{no swap}\rangle$
	→	$\|3\rangle\|0\rangle$	→	$\|0\rangle\|3\rangle\|\text{swap}\rangle$	→	$\|0\rangle\|3\rangle\|\text{swap}\rangle$
	→	$\|3\rangle\|1\rangle$	→	$\|1\rangle\|3\rangle\|\text{swap}\rangle$	→	$\|1\rangle\|3\rangle\|\text{swap}\rangle$
	→	$\|3\rangle\|2\rangle$	→	$\|2\rangle\|3\rangle\|\text{swap}\rangle$	→	$\|2\rangle\|3\rangle\|\text{swap}\rangle$
	→	$\|3\rangle\|3\rangle$	→	$\|3\rangle\|3\rangle\|\text{no swap}\rangle$	→	~~$\|3\rangle\|3\rangle\|\text{no swap}\rangle$~~

Create a uniform superposition

*Up to normalization

Antisymmetrization via a Quantum Sort

	$\rightarrow$	$\|0\rangle\,\|0\rangle$	$\rightarrow$	$\|0\rangle\,\|0\rangle\,\|\text{no swap}\rangle$	$\rightarrow$	~~$\|0\rangle\,\|0\rangle\,\|\text{no swap}\rangle$~~
	$\rightarrow$	$\|0\rangle\,\|1\rangle$	$\rightarrow$	$\|0\rangle\,\|1\rangle\,\|\text{no swap}\rangle$	$\rightarrow$	$\|0\rangle\,\|1\rangle\,\|\text{no swap}\rangle$
	$\rightarrow$	$\|0\rangle\,\|2\rangle$	$\rightarrow$	$\|0\rangle\,\|2\rangle\,\|\text{no swap}\rangle$	$\rightarrow$	$\|0\rangle\,\|2\rangle\,\|\text{no swap}\rangle$
	$\rightarrow$	$\|0\rangle\,\|3\rangle$	$\rightarrow$	$\|0\rangle\,\|3\rangle\,\|\text{no swap}\rangle$	$\rightarrow$	$\|0\rangle\,\|3\rangle\,\|\text{no swap}\rangle$
	$\rightarrow$	$\|1\rangle\,\|0\rangle$	$\rightarrow$	$\|0\rangle\,\|1\rangle\,\|\text{swap}\rangle$	$\rightarrow$	$\|0\rangle\,\|1\rangle\,\|\text{swap}\rangle$
	$\rightarrow$	$\|1\rangle\,\|1\rangle$	$\rightarrow$	$\|1\rangle\,\|1\rangle\,\|\text{no swap}\rangle$	$\rightarrow$	~~$\|1\rangle\,\|1\rangle\,\|\text{no swap}\rangle$~~
	$\rightarrow$	$\|1\rangle\,\|2\rangle$	$\rightarrow$	$\|1\rangle\,\|2\rangle\,\|\text{no swap}\rangle$	$\rightarrow$	$\|1\rangle\,\|2\rangle\,\|\text{no swap}\rangle$
	$\rightarrow$	$\|1\rangle\,\|3\rangle$	$\rightarrow$	$\|1\rangle\,\|3\rangle\,\|\text{no swap}\rangle$	$\rightarrow$	$\|1\rangle\,\|3\rangle\,\|\text{no swap}\rangle$
$\|0\rangle\,\|0\rangle$	$\rightarrow$	$\|2\rangle\,\|0\rangle$	$\rightarrow$	$\|0\rangle\,\|2\rangle\,\|\text{swap}\rangle$	$\rightarrow$	$\|0\rangle\,\|2\rangle\,\|\text{swap}\rangle$
	$\rightarrow$	$\|2\rangle\,\|1\rangle$	$\rightarrow$	$\|1\rangle\,\|2\rangle\,\|\text{swap}\rangle$	$\rightarrow$	$\|1\rangle\,\|2\rangle\,\|\text{swap}\rangle$
	$\rightarrow$	$\|2\rangle\,\|2\rangle$	$\rightarrow$	$\|2\rangle\,\|2\rangle\,\|\text{no swap}\rangle$	$\rightarrow$	~~$\|2\rangle\,\|2\rangle\,\|\text{no swap}\rangle$~~
	$\rightarrow$	$\|2\rangle\,\|3\rangle$	$\rightarrow$	$\|2\rangle\,\|3\rangle\,\|\text{no swap}\rangle$	$\rightarrow$	$\|2\rangle\,\|3\rangle\,\|\text{no swap}\rangle$
	$\rightarrow$	$\|3\rangle\,\|0\rangle$	$\rightarrow$	$\|0\rangle\,\|3\rangle\,\|\text{swap}\rangle$	$\rightarrow$	$\|0\rangle\,\|3\rangle\,\|\text{swap}\rangle$
	$\rightarrow$	$\|3\rangle\,\|1\rangle$	$\rightarrow$	$\|1\rangle\,\|3\rangle\,\|\text{swap}\rangle$	$\rightarrow$	$\|1\rangle\,\|3\rangle\,\|\text{swap}\rangle$
	$\rightarrow$	$\|3\rangle\,\|2\rangle$	$\rightarrow$	$\|2\rangle\,\|3\rangle\,\|\text{swap}\rangle$	$\rightarrow$	$\|2\rangle\,\|3\rangle\,\|\text{swap}\rangle$
	$\rightarrow$	$\|3\rangle\,\|3\rangle$	$\rightarrow$	$\|3\rangle\,\|3\rangle\,\|\text{no swap}\rangle$	$\rightarrow$	~~$\|3\rangle\,\|3\rangle\,\|\text{no swap}\rangle$~~

Sort registers and
record swaps

Antisymmetrization via a Quantum Sort

	$\rightarrow$	$\|0\rangle\ \|0\rangle$	$\rightarrow$	$\|0\rangle\ \|0\rangle\ \|\text{no swap}\rangle$	$\rightarrow$	~~$\|0\rangle\ \|0\rangle\ \|\text{no swap}\rangle$~~
	$\rightarrow$	$\|0\rangle\ \|1\rangle$	$\rightarrow$	$\|0\rangle\ \|1\rangle\ \|\text{no swap}\rangle$	$\rightarrow$	$\|0\rangle\ \|1\rangle\ \|\text{no swap}\rangle$
	$\rightarrow$	$\|0\rangle\ \|2\rangle$	$\rightarrow$	$\|0\rangle\ \|2\rangle\ \|\text{no swap}\rangle$	$\rightarrow$	$\|0\rangle\ \|2\rangle\ \|\text{no swap}\rangle$
	$\rightarrow$	$\|0\rangle\ \|3\rangle$	$\rightarrow$	$\|0\rangle\ \|3\rangle\ \|\text{no swap}\rangle$	$\rightarrow$	$\|0\rangle\ \|3\rangle\ \|\text{no swap}\rangle$
	$\rightarrow$	$\|1\rangle\ \|0\rangle$	$\rightarrow$	$\|0\rangle\ \|1\rangle\ \|\text{swap}\rangle$	$\rightarrow$	$\|0\rangle\ \|1\rangle\ \|\text{swap}\rangle$
	$\rightarrow$	$\|1\rangle\ \|1\rangle$	$\rightarrow$	$\|1\rangle\ \|1\rangle\ \|\text{no swap}\rangle$	$\rightarrow$	~~$\|1\rangle\ \|1\rangle\ \|\text{no swap}\rangle$~~
	$\rightarrow$	$\|1\rangle\ \|2\rangle$	$\rightarrow$	$\|1\rangle\ \|2\rangle\ \|\text{no swap}\rangle$	$\rightarrow$	$\|1\rangle\ \|2\rangle\ \|\text{no swap}\rangle$
	$\rightarrow$	$\|1\rangle\ \|3\rangle$	$\rightarrow$	$\|1\rangle\ \|3\rangle\ \|\text{no swap}\rangle$	$\rightarrow$	$\|1\rangle\ \|3\rangle\ \|\text{no swap}\rangle$
$\|0\rangle\ \|0\rangle$	$\rightarrow$	$\|2\rangle\ \|0\rangle$	$\rightarrow$	$\|0\rangle\ \|2\rangle\ \|\text{swap}\rangle$	$\rightarrow$	$\|0\rangle\ \|2\rangle\ \|\text{swap}\rangle$
	$\rightarrow$	$\|2\rangle\ \|1\rangle$	$\rightarrow$	$\|1\rangle\ \|2\rangle\ \|\text{swap}\rangle$	$\rightarrow$	$\|1\rangle\ \|2\rangle\ \|\text{swap}\rangle$
	$\rightarrow$	$\|2\rangle\ \|2\rangle$	$\rightarrow$	$\|2\rangle\ \|2\rangle\ \|\text{no swap}\rangle$	$\rightarrow$	~~$\|2\rangle\ \|2\rangle\ \|\text{no swap}\rangle$~~
	$\rightarrow$	$\|2\rangle\ \|3\rangle$	$\rightarrow$	$\|2\rangle\ \|3\rangle\ \|\text{no swap}\rangle$	$\rightarrow$	$\|2\rangle\ \|3\rangle\ \|\text{no swap}\rangle$
	$\rightarrow$	$\|3\rangle\ \|0\rangle$	$\rightarrow$	$\|0\rangle\ \|3\rangle\ \|\text{swap}\rangle$	$\rightarrow$	$\|0\rangle\ \|3\rangle\ \|\text{swap}\rangle$
	$\rightarrow$	$\|3\rangle\ \|1\rangle$	$\rightarrow$	$\|1\rangle\ \|3\rangle\ \|\text{swap}\rangle$	$\rightarrow$	$\|1\rangle\ \|3\rangle\ \|\text{swap}\rangle$
	$\rightarrow$	$\|3\rangle\ \|2\rangle$	$\rightarrow$	$\|2\rangle\ \|3\rangle\ \|\text{swap}\rangle$	$\rightarrow$	$\|2\rangle\ \|3\rangle\ \|\text{swap}\rangle$
	$\rightarrow$	$\|3\rangle\ \|3\rangle$	$\rightarrow$	$\|3\rangle\ \|3\rangle\ \|\text{no swap}\rangle$	$\rightarrow$	~~$\|3\rangle\ \|3\rangle\ \|\text{no swap}\rangle$~~

Flag and delete repetitions

Antisymmetrization via a Quantum Sort

$$
\begin{array}{cccccccc}
 & \rightarrow & |0\rangle\,|0\rangle & \rightarrow & |0\rangle\,|0\rangle\,|\text{no swap}\rangle & \rightarrow & \cancel{|0\rangle\,|0\rangle\,|\text{no swap}\rangle} \\
 & \rightarrow & |0\rangle\,|1\rangle & \rightarrow & |0\rangle\,|1\rangle\,|\text{no swap}\rangle & \rightarrow & |0\rangle\,|1\rangle\,|\text{no swap}\rangle \\
 & \rightarrow & |0\rangle\,|2\rangle & \rightarrow & |0\rangle\,|2\rangle\,|\text{no swap}\rangle & \rightarrow & |0\rangle\,|2\rangle\,|\text{no swap}\rangle \\
 & \rightarrow & |0\rangle\,|3\rangle & \rightarrow & |0\rangle\,|3\rangle\,|\text{no swap}\rangle & \rightarrow & |0\rangle\,|3\rangle\,|\text{no swap}\rangle \\
 & \rightarrow & |1\rangle\,|0\rangle & \rightarrow & |0\rangle\,|1\rangle\,|\text{swap}\rangle & \rightarrow & |0\rangle\,|1\rangle\,|\text{swap}\rangle \\
 & \rightarrow & |1\rangle\,|1\rangle & \rightarrow & |1\rangle\,|1\rangle\,|\text{no swap}\rangle & \rightarrow & \cancel{|1\rangle\,|1\rangle\,|\text{no swap}\rangle} \\
 & \rightarrow & |1\rangle\,|2\rangle & \rightarrow & |1\rangle\,|2\rangle\,|\text{no swap}\rangle & \rightarrow & |1\rangle\,|2\rangle\,|\text{no swap}\rangle \\
 & \rightarrow & |1\rangle\,|3\rangle & \rightarrow & |1\rangle\,|3\rangle\,|\text{no swap}\rangle & \rightarrow & |1\rangle\,|3\rangle\,|\text{no swap}\rangle \\
|0\rangle\,|0\rangle & \rightarrow & |2\rangle\,|0\rangle & \rightarrow & |0\rangle\,|2\rangle\,|\text{swap}\rangle & \rightarrow & |0\rangle\,|2\rangle\,|\text{swap}\rangle \\
 & \rightarrow & |2\rangle\,|1\rangle & \rightarrow & |1\rangle\,|2\rangle\,|\text{swap}\rangle & \rightarrow & |1\rangle\,|2\rangle\,|\text{swap}\rangle \\
 & \rightarrow & |2\rangle\,|2\rangle & \rightarrow & |2\rangle\,|2\rangle\,|\text{no swap}\rangle & \rightarrow & \cancel{|2\rangle\,|2\rangle\,|\text{no swap}\rangle} \\
 & \rightarrow & |2\rangle\,|3\rangle & \rightarrow & |2\rangle\,|3\rangle\,|\text{no swap}\rangle & \rightarrow & |2\rangle\,|3\rangle\,|\text{swap}\rangle \\
 & \rightarrow & |3\rangle\,|0\rangle & \rightarrow & |0\rangle\,|3\rangle\,|\text{swap}\rangle & \rightarrow & |0\rangle\,|3\rangle\,|\text{swap}\rangle \\
 & \rightarrow & |3\rangle\,|1\rangle & \rightarrow & |1\rangle\,|3\rangle\,|\text{swap}\rangle & \rightarrow & |1\rangle\,|3\rangle\,|\text{swap}\rangle \\
 & \rightarrow & |3\rangle\,|2\rangle & \rightarrow & |2\rangle\,|3\rangle\,|\text{swap}\rangle & \rightarrow & |2\rangle\,|3\rangle\,|\text{swap}\rangle \\
 & \rightarrow & |3\rangle\,|3\rangle & \rightarrow & |3\rangle\,|3\rangle\,|\text{no swap}\rangle & \rightarrow & \cancel{|3\rangle\,|3\rangle\,|\text{no swap}\rangle}
\end{array}
$$

Outcome:

$$
\Big(|0\rangle\,|1\rangle+|0\rangle\,|2\rangle+|0\rangle\,|3\rangle+|1\rangle\,|2\rangle+|1\rangle\,|3\rangle+|2\rangle\,|3\rangle\Big)\otimes\Big(|\text{swap}\rangle+|\text{no swap}\rangle\Big)
$$

Antisymmetrization via a Quantum Sort

Discard the sorted data register and use the register with swaps to (anti)symmetrize a given state

$$\Big(|4\rangle\,|7\rangle \Big)\Big(|\text{swap}\rangle + |\text{no swap}\rangle \Big) \rightarrow \Big(|4\rangle\,|7\rangle + |7\rangle\,|4\rangle \Big)\,|0\rangle$$

by running the sort backwards. The comparisons in the sort will clean the ancillae encoding swaps.

Results

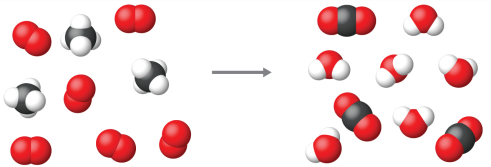
Complexity:

- $\mathcal{O}(m \log^2 m \log N)$ gates (prior: $\mathcal{O}(m^2 \log^2 N)$)
- $\mathcal{O}(\log^2 m \log \log N)$ depth (prior: $\mathcal{O}(m^2 \log^2 N)$)
- polynomial and exponential improvement to Abrams & Lloyd

Simulating time-dependent Hamiltonians

Motivation: Simulating Quantum Systems is Notoriously Difficult

First application of quantum computing



Product formulae: [Lloyd 1996, Aharonov & Ta-Shma 2003, Berry et al. 2007, Wiebe 2010, Campbell 2018, ...]

LCU: [Childs & Wiebe 2012, Berry et al. 2013, Berry et al. 2014, Berry et al. 2015, Berry et al. 2017, ...]

Other: [Childs 2010, Berry & Childs 2009, Low & Chuang 2016, Low & Chuang 2017, Low & Wiebe 2018, Gilyén 2019, ...]

+ simulations of special Hamiltonians, resource studies, applications

Time-dependent Hamiltonian Simulation

Implement the time evolution

$$i \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle$$

with logical error at most ϵ where H is a d-sparse Hermitian matrix.

[Lloyd 1996, Aharonov & Ta-Shma 2003, Wiebe et al. 2011, Poulin et al. 2011, Low & Wiebe 2018, Berry et al. 2019]

NEW: Algorithm for simulating time-dependent Hamiltonians with poly-logarithmic dependence on the inverse error.

Application: Interaction Picture Simulation

Reduced dependence on the norm in exchange for a time-dependent Hamiltonian

$$H = A + B$$

A – large norm, easy to implement, for example diagonal

B – small norm, must use regular Hamiltonian simulation methods

$$H_I(t) = e^{iAt} B e^{-iAt}$$

[Low, Wiebe 2019]

Discretization

- Split the evolution into r segments
- Truncated Dyson (Taylor) series

$$U(0, T/r) \approx \sum_{k=0}^{K} \frac{(-i)^k}{k!} \mathcal{T} \int_0^{T/r} d\mathbf{t}\, H(t_k) \dots H(t_1)$$

- Discretize the integrals

$$U(0, T/r) \approx \sum_{k=0}^{K} \frac{(-iT/r)^k}{M^k k!} \sum_{j_1,\dots,j_k=0}^{M-1} \mathcal{T} H(t_{j_k}) \dots H(t_{j_1})$$

- Decompose Hamiltonians into linear combinations of unitaries H_ℓ

$$H(t) = \gamma \sum_{\ell=0}^{L-1} H_\ell(t) \qquad \text{or} \qquad H(t) = \sum_{\ell=0}^{L-1} \alpha_\ell(t) H_\ell$$

LCU for Hamiltonian Simulation

The evolution can be approximated by a linear combination of unitaries

$$U(0, T/r) \approx \sum_j \beta_j V_j,$$

where β_j-s are the coefficients and V_j-s products of unitaries. $U(0, T/r)$ is implemented through

and then boosted to almost perfect success rate using oblivious amplitude amplification.

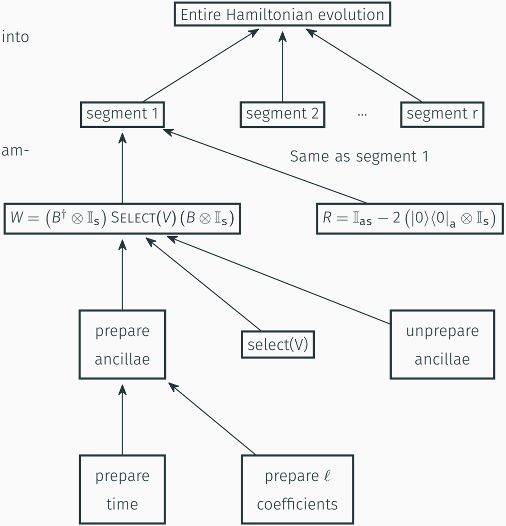
Overview

Divide the evolution into segments

Oblivious amplitude amplification

Circuits in the paper/thesis

State preparation



[Berry et al. 2014, Kieferova et al. 2019]

How Do We Enforce the Correct Order of Unitaries?

The times for the Hamiltonians must come in the correct order

$$\mathcal{T} H(t_{j_k}) \dots H(t_{j_2}) H(t_{j_1}).$$

NEW: Two approaches to create a "clock" register.

Ordering based on sorting:

- value of k in unary
- create $\sum_i t_i \otimes \cdots \otimes \sum_i t_i$
- sort the registers

Results

Complexity:

- $\mathcal{O}\left(d^2 H_{\max} T \frac{\log(dH_{\max}T/\epsilon)}{\log\log(dH_{\max}T/\epsilon)}\right)$ queries, same as for the time-independent LCU algorithm

  [Lloyd 1996, Aharonov 2003, Aharonov 2008, Wiebe et al. 2011, Poulin 2011] $\sim$ $poly(1/\epsilon)$

- gate complexity depends on $\log(||\dot{H}||)$

  ([Lloyd 1996, Aharonov 2003, Aharonov 2008, Wiebe et al. 2011] polynomial dependence,

  [Poulin 2011] independent)

Summary

- An efficient, low-depth algorithm for antisymmetrization of a fermionic wavefunction.
- A new algorithm simulating time-dependent Hamiltonians.

Thank you!