Some improvements to product formula circuits for Hamiltonian simulation

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A crash course in chemistry

Calculus. Differential equation $y' = ay$. Solution $y = y_0\, e^{at}$.

Linear algebra. Diff. equation $v' = Av$. Solution $v = e^{At} v_0$.

Fun fact: $e^X = I + X + \frac{X^2}{2} + \frac{X^3}{3!} + \ldots$.

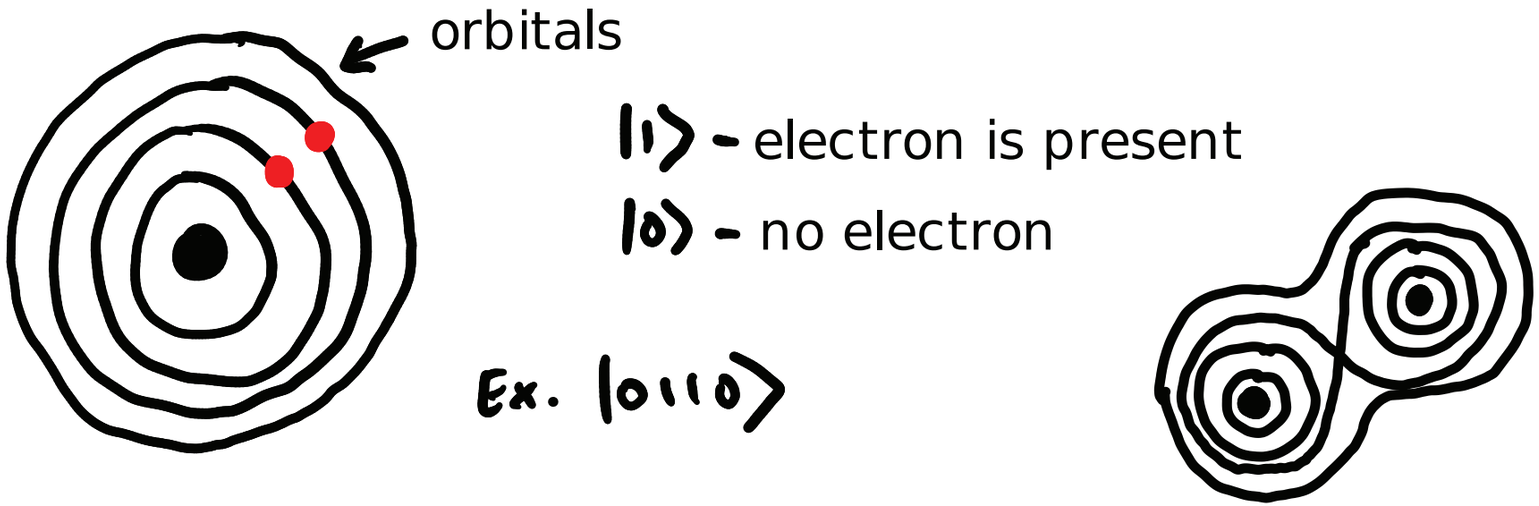
Physics. Diff. equation $v' = -iHv$. Solution $v = e^{-iHt} v_0$.

Fun fact: If H is hermitian, then e^{-iHt} is unitary.

The equation (in appropriate units) is called the *Schrödinger equation*. H is called the *Hamiltonian*.

A crash course in chemistry, continued

Chemistry.



Fun fact: Orbits are not actually circles. They are spherical harmonics.

A crash course in chemistry, continued

Chemistry.

The Hamiltonian for chemistry takes the form

$$H = \sum_{p,q} h_{pq}\, a_p^\dagger\, a_q + \sum_{p,q,r,s} h_{pqrs}\, a_p^\dagger\, a_q^\dagger\, a_r\, a_s.$$

Example: The term $h(a_0^\dagger\, a_1 + a_1^\dagger\, a_0)$ means:
An electron can jump from orbital 0 to orbital 1 (or vice versa).
Moreover, this happens with "probability per second" h.

Example: The term $h(a_0^\dagger\, a_1^\dagger\, a_2\, a_0 + a_0^\dagger\, a_2^\dagger\, a_1\, a_0)$ means:
An electron can jump from orbital 1 to orbital 2 (or vice versa), but only if orbital 0 is occupied.

Fun fact: all elementary laws of nature involve at most 2 particles.

A crash course in chemistry, continued

Chemistry.

The Hamiltonian for chemistry takes the form

$$H = \sum_{p,q} h_{pq}\, a_p^\dagger\, a_q + \sum_{p,q,r,s} h_{pqrs}\, a_p^\dagger\, a_q^\dagger\, a_r\, a_s.$$

Here:

$$a_p = Z \otimes \ldots \otimes Z \otimes \overset{p}{\underset{\downarrow}{A}} \otimes I \otimes \ldots \otimes I. \qquad \text{“Jordan-Wigner transform”}$$

$$A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \;=\; |0\rangle\langle 1| \qquad \text{“annihilation operator”}$$

Example: $a_2^\dagger a_5 = (Z \otimes Z \otimes A^\dagger \otimes I \otimes I \otimes I)(Z \otimes Z \otimes Z \otimes Z \otimes Z \otimes A) = I \otimes I \otimes A^\dagger \otimes Z \otimes Z \otimes A.$

Product formula circuits for Hamiltonian simulation

Fun fact: If A and B commute, then $e^{A+B} = e^A e^B$.

If A and B don't commute, in general $e^{A+B} \neq e^A e^B$.

However, if $A, B \approx I$, then $e^{A+B} \approx e^A e^B$.

We have $e^{A+B} = \lim_{n\to\infty} (e^{A/n} e^{B/n})^n$

Given: Hamiltonian $H = \sum \ldots$, time t.

Want: Quantum circuit that implements $U = e^{-iHt}$ up to epsilon.

Trotter-Suzuki method (product formula method): Divide t into small enough intervals and pretend that

$$e^{\epsilon(A_1+\ldots+A_k)} = e^{\epsilon A_1} \ldots e^{\epsilon A_k}.$$

Hamiltonian "templates"

Example: Find a circuit for $e^{-i\theta\,(a_0^\dagger\, a_5^\dagger\, a_8\, a_3 + a_3^\dagger\, a_8^\dagger\, a_5\, a_0)}$

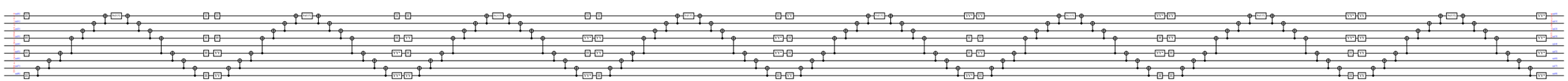
Naive method: sum of Paulis, using $A = \frac{1}{2}(X + iY)$ and $A^\dagger = \frac{1}{2}(X - iY)$.

We have: $a_0^\dagger\, a_5^\dagger\, a_8\, a_3 + a_3^\dagger\, a_8^\dagger\, a_5\, a_0$

$= A^\dagger ZZAIA^\dagger ZZA + AZZA^\dagger IAZZA^\dagger$

$= \frac{1}{16}(\ (X - iY)ZZ(X + iY)I(X - iY)ZZ(X + iY)\ \ +\ \ (X - iY)ZZ(X + iY)I(X - iY)ZZ(X + iY)\ )$

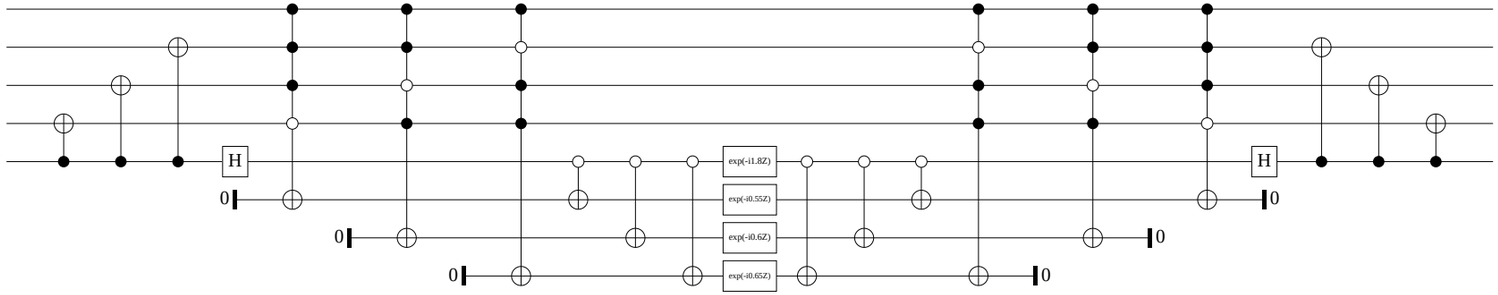
$= \frac{1}{8}\ (\ XZZXIXZZX + XZZXIYZZY - XZZYIXZZY + XZZYIYZZX$
$\quad +YZZXIXZZY - YZZXIYZZX + YZZYIXZZX + YZZYIYZZY\ )$



Improvements, part 1

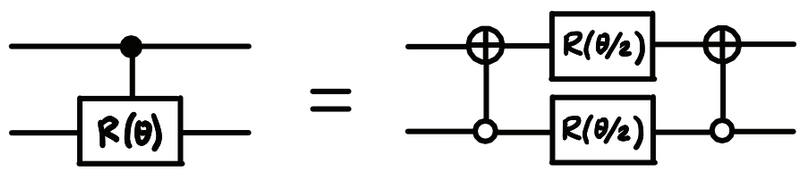
- Better circuit templates. The following implements

$$\begin{aligned} &\phi_1 \left(a_0^\dagger a_5^\dagger a_8 a_3 + a_3^\dagger a_8^\dagger a_5 a_0\right) \\ +\,&\phi_2 \left(a_0^\dagger a_8^\dagger a_5 a_3 + a_3^\dagger a_5^\dagger a_8 a_0\right) \\ +\,&\phi_3 \left(a_0^\dagger a_3^\dagger a_8 a_5 + a_5^\dagger a_8^\dagger a_3 a_0\right) \end{aligned}$$

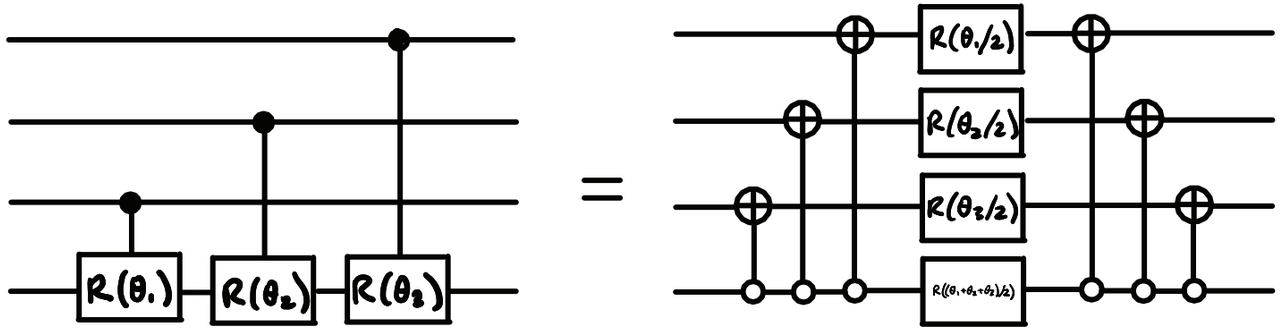


Note: 3 times the number of Hamiltonian terms at 1/8 of the depth.

Controlled rotation gate:

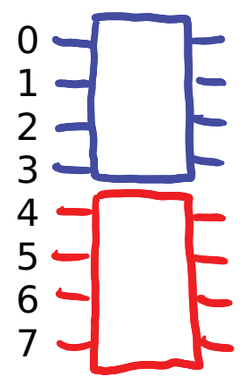


Multiple controlled rotations:

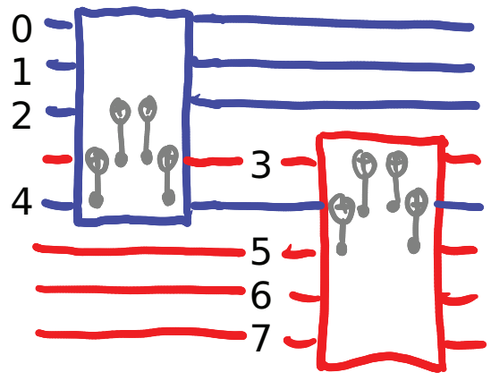


Improvements, part 2: Skilift parallelization

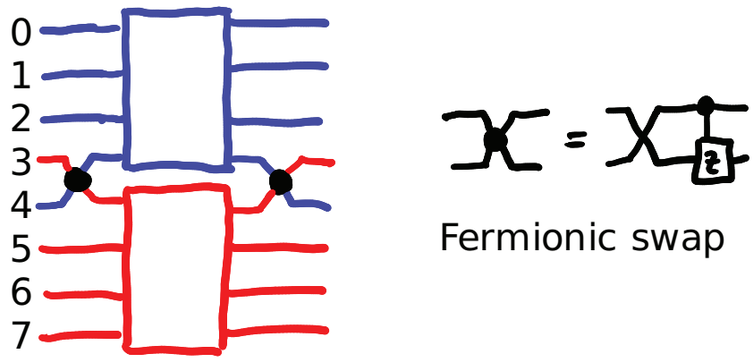
- A template at orbitals 0,1,2,3 and a template at orbitals 4,5,6,7 don't overlap and can be done in parallel.



- Problem: Templates at 0,1,2,4 and 3,5,6,7 also commute, but can't be done in parallel because they overlap.



- Solution: Fermionic swap



Fermionic swap

Mathematical problem: Repeatedly permute the orbitals so that each 4-tuple occurs at least once. What is the shortest* sequence of such permutations? Also, the permutations should be low depth.

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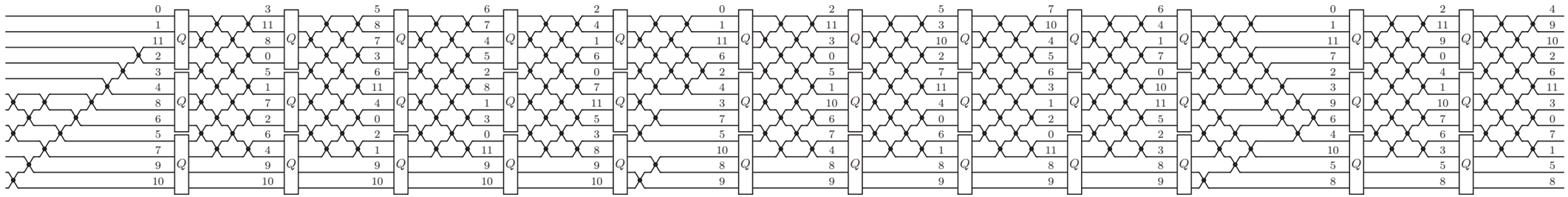
Solution: Andre Kornell, with help from Nazarov and Speyer:

- Based on *Mobius transformations* over a finite field.
- Within a factor of 1.5 of optimal*.
- Average permutation depth per stage is constant.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5 8 7 3 6 11 4 0 2 1 9 10
6 7 4 5 2 8 1 3 0 11 9 10
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0 1 11 6 2 4 3 7 5 10 8 9
2 11 3 0 5 1 10 6 7 4 8 9
5 3 10 2 7 11 4 6 0 1 8 9
7 10 4 5 6 3 1 2 0 11 8 9
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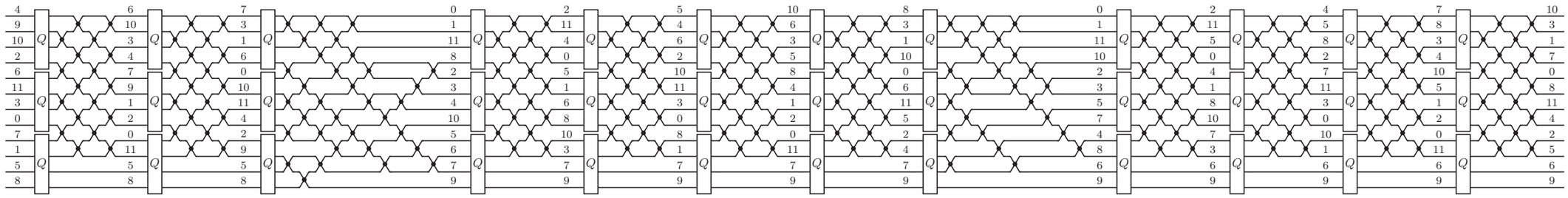
4 9 10 2 6 11 3 6 10 3 4 7 9 1 2 0 11 5 8
6 10 3 4 7 9 1 2 0 11 5 8
7 3 1 6 0 10 11 4 2 9 5 8
0 1 11 8 2 3 4 10 5 6 7 9
2 11 4 0 5 1 6 8 10 3 7 9
5 4 6 2 10 11 3 0 8 1 7 9
10 6 3 5 8 4 1 2 0 7 11 9
8 3 1 10 0 6 11 5 2 4 7 9
0 1 11 10 2 3 5 7 4 8 6 9
2 11 5 0 4 1 8 10 7 3 6 9
4 5 8 2 7 11 3 0 10 1 6 9
7 8 3 4 10 5 1 2 0 11 6 9
10 3 1 7 0 10 11 5 2 9 6 9
10 3 1 7 0 8 11 4 6 5 9
3 2 6 0 5 1 9 11 8 4 7 10
5 6 9 3 8 2 4 0 11 1 7 10
8 9 4 5 11 6 1 3 0 2 7 10
11 4 1 8 0 9 2 5 3 6 7 10
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2 4 9 0 6 1 7 11 5 3 8 10
6 9 7 2 5 4 3 0 11 1 8 10
5 7 3 6 11 9 1 2 0 4 8 10
11 3 1 5 0 7 4 6 2 9 8 10
0 1 5 11 2 3 8 10 4 7 6 9
2 5 8 0 4 1 7 11 10 3 6 9
4 8 7 2 10 11 3 0 1 6 9 9

Mobius transformations

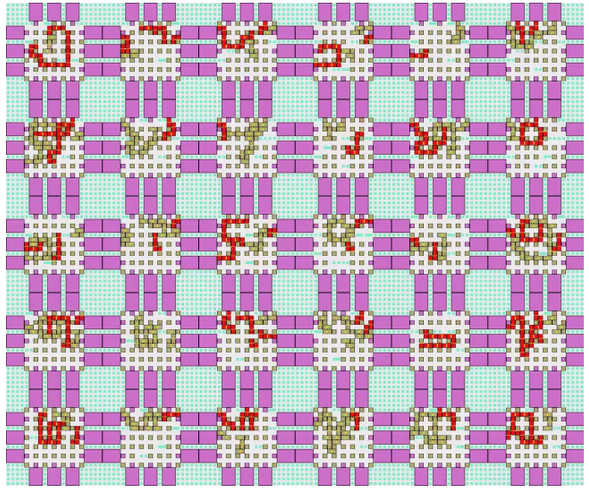
- Functions of the form $f(z) = \dfrac{az + b}{cz + d}$.
- Usually defined on $\mathbb{C} \cup \{\infty\}$, but also works on $\mathbb{Z}_p \cup \{\infty\}$ for a finite field.
- Property: 3-transitivity: 3 points determine the whole map.
- Property: when it swaps two points, it's an involution.
- A Mobius transformation that's an involution determines a pairing; each pair of pairs appears in exactly one such pairing.

Down the toolchain

After optimizing the logical circuit, we compiled it all the way down to lattice surgery on a lattice of iron traps. [Christopher Dean and Tyler LeBlond].

Error correction cycle time: 64 cycles per second. (Note: superconducting is about 1000 times faster, but this is iron traps).

The following movie is in real time.



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This research was supported under DARPA Research Contract HR001122C0066.