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

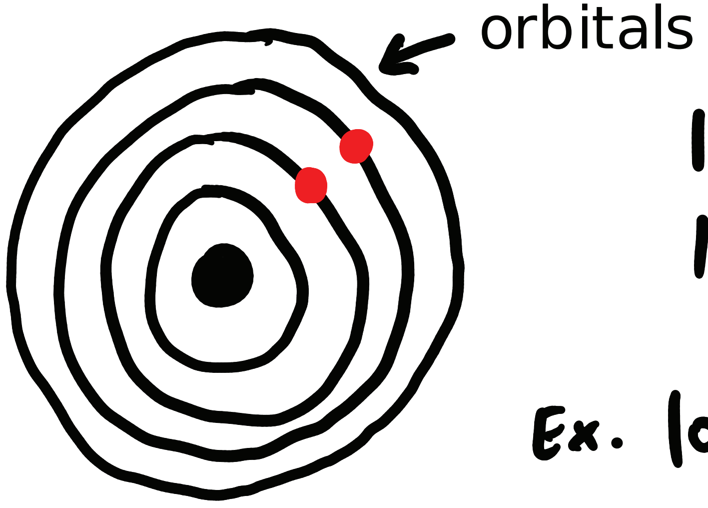
Physics. Diff. equation $v' = -iHv$. Solution $v = e^{-iHt} v_0$.

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

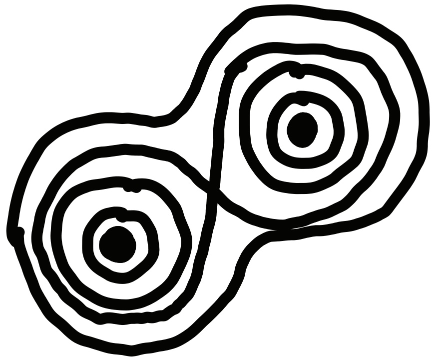
Chemistry.



$|1\rangle$ - electron is present

$|0\rangle$ - no electron

Ex. $|0110\rangle$



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:

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

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

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 $e^{-i\theta\,(a_0^\dagger\, a_5^\dagger\, a_8\, a_3 + a_3^\dagger\, a_8^\dagger\, a_5\, a_0)}$

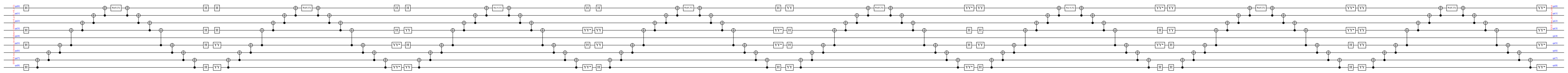
Naive method: sum of Paulis, using $A = \frac{1}{2}(X + iY)$ and $A^\dagger = \frac{1}{2}(X - iY)$.

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

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

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

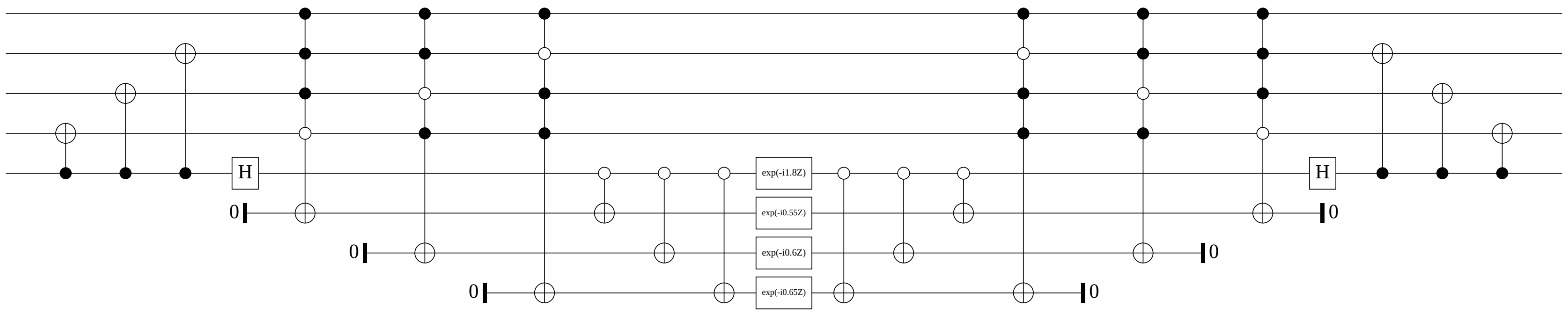
$= \frac{1}{8}\ (\ XZZXIXZZX + XZZXIYZZY - XZZYIXZZY + XZZYIYZZX$
$+YZZXIXZZY - YZZXIYZZX + YZZYIXZZX + YZZYIYZZY\ )$



Improvements, part 1

- Better circuit templates. The following implements

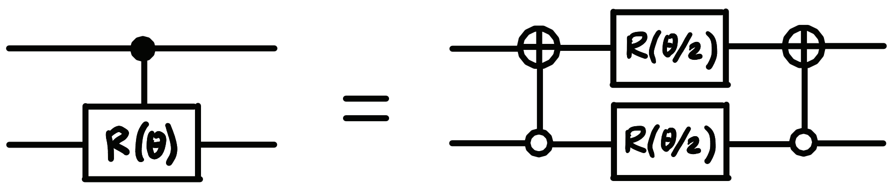
$$\begin{aligned} & \phi_1\,(a_0^\dagger\, a_5^\dagger\, a_8\, a_3 + a_3^\dagger\, a_8^\dagger\, a_5\, a_0) \\ + & \phi_2\,(a_0^\dagger\, a_8^\dagger\, a_5\, a_3 + a_3^\dagger\, a_5^\dagger\, a_8\, a_0) \\ + & \phi_3\,(a_0^\dagger\, a_3^\dagger\, a_8\, a_5 + a_5^\dagger\, a_8^\dagger\, a_3\, a_0) \end{aligned}$$

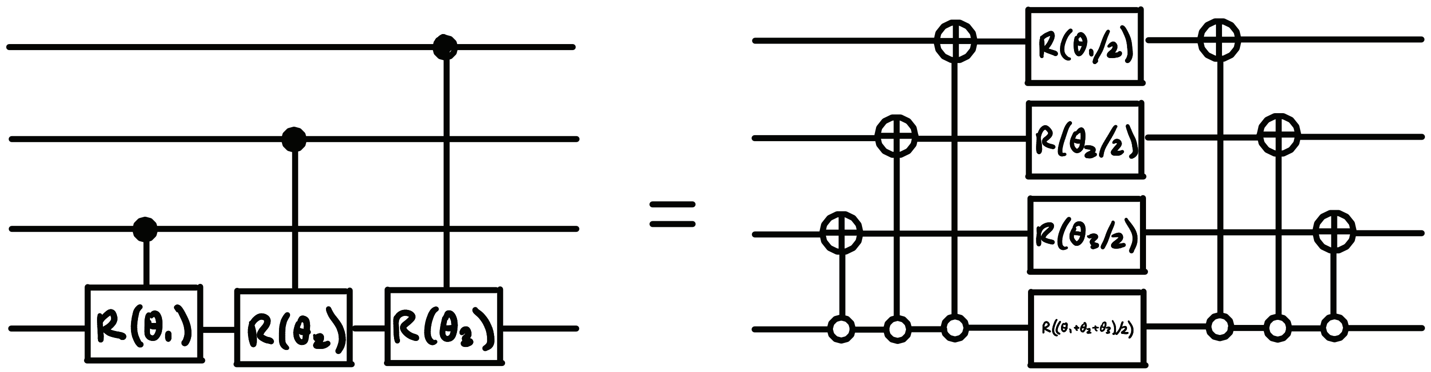


Note: 3 times the number of Hamiltonian terms at 1/8 of the depth.

Controlled rotation gate:

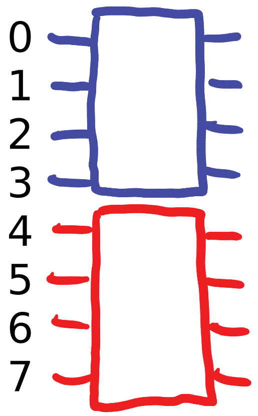
Multiple controlled rotations:



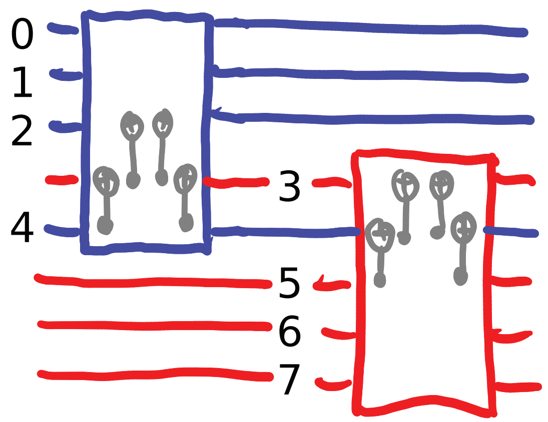


Improvements, part 2: Skilift parallelization

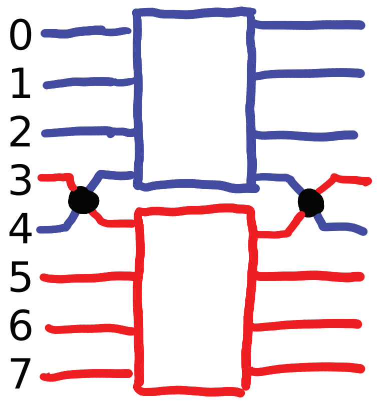
- A template at orbitals 0,1,2,3 and a template at orbitals 4,5,6,7 don't overlap and can be done in parallel.

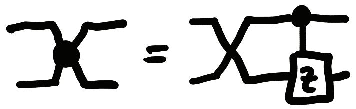


- Problem: Templates at 0,1,2,4 and 3,5,6,7 also commute, but can't be done in parallel because they overlap.



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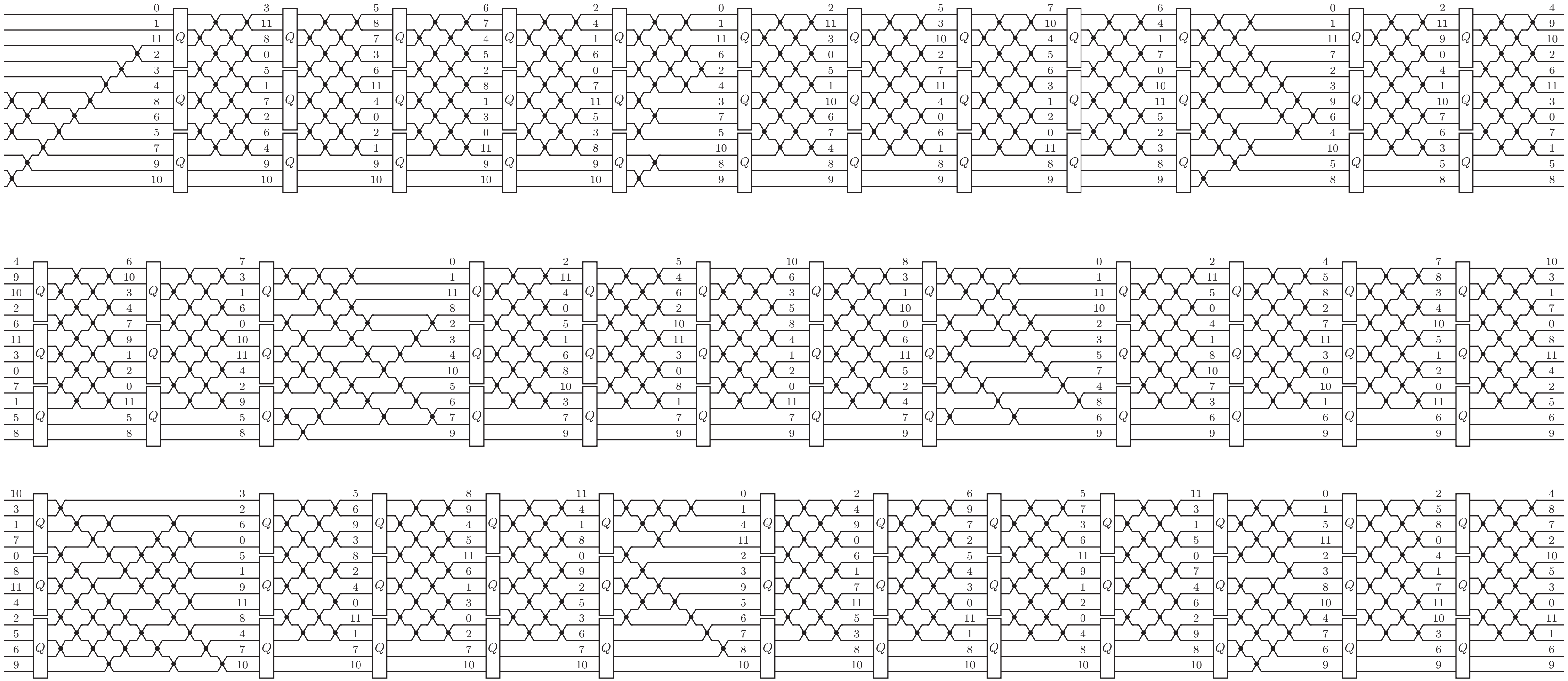
Solution: Andre Kornell, with help from Nazarov and Speyer:

- Based on *Mobius transformations* over a finite field.
- Within a factor of 1.5 of optimal*.
- Average permutation depth per stage is constant.



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.