CAN ONE DO QUANTUM CHEMISTRY WITH A SMALL QUANTUM COMPUTER?

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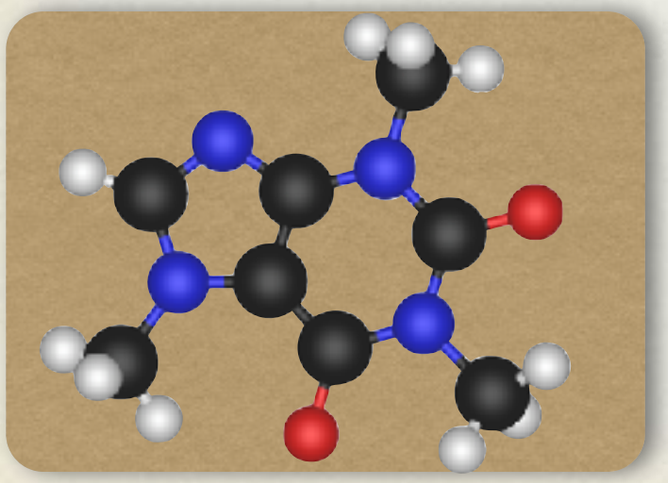
Aspen Quantum Algorithms

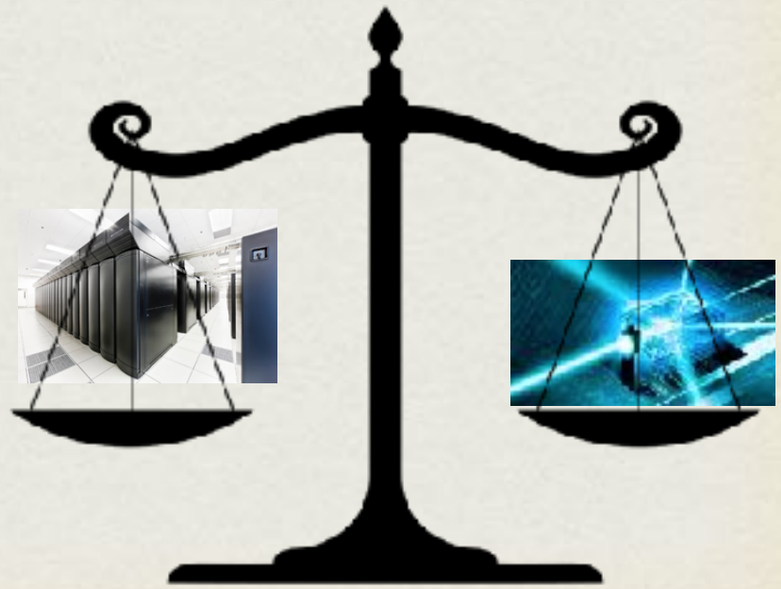
I want to simulate quantum systems.

I have a big classical computer.

Soon we'll have ~100 qubit quantum computer that can run for a day (hey, I'm optimistic)

When should I use my classical computer, my small quantum computer, and when is it hopeless?





Algorithms

Quantum Algorithms

Exact classical algorithms

Approximate classical algorithms

Simulating quantum mechanical ground states:

- Hermitian Matrix H
- has some ground state Ψ_0
- with some ground state energy E_0
- which we want to approximate to a (chemical) accuracy.

$$e^{iTH}|\Psi_i\rangle = |\Psi[T]\rangle$$

$e^{-TH}|\Psi_i\rangle = |\Psi_0\rangle$ dissipative.

The quantum chemistry Hamiltonian:

$$H = \sum_{pq} t_{pq} c_p^\dagger c_q + \frac{1}{2} \sum_{pqrs} V_{pqrs} c_p^\dagger c_q^\dagger c_r c_s$$

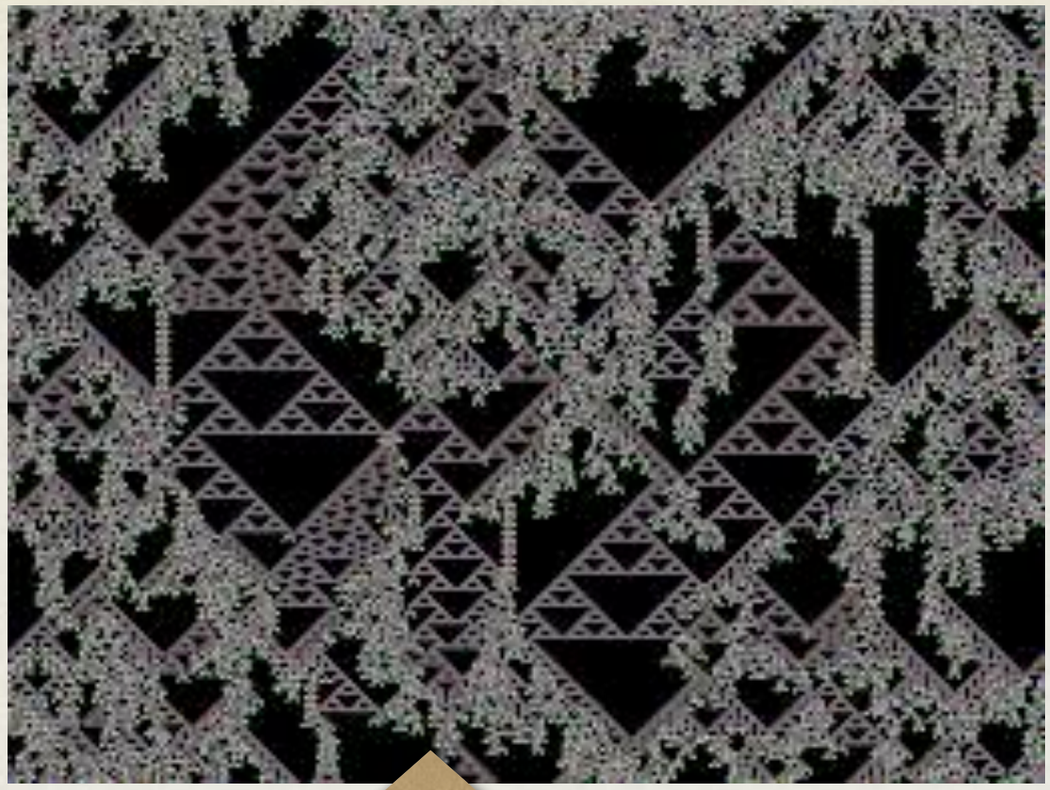
Calculated once per molecule

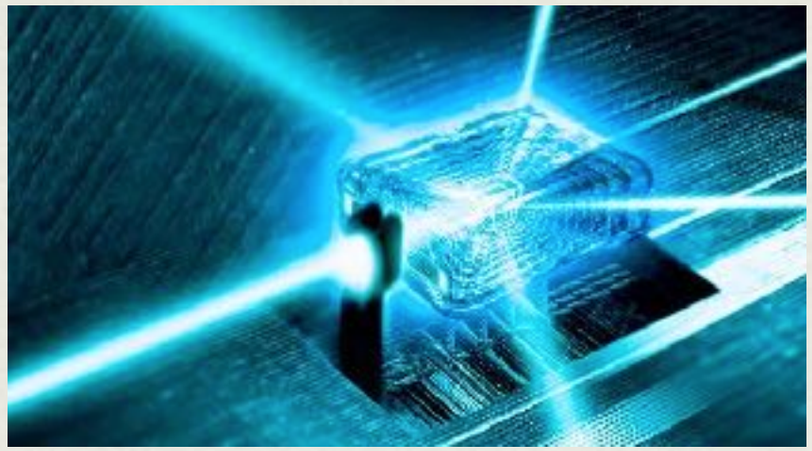
N^4 numbers

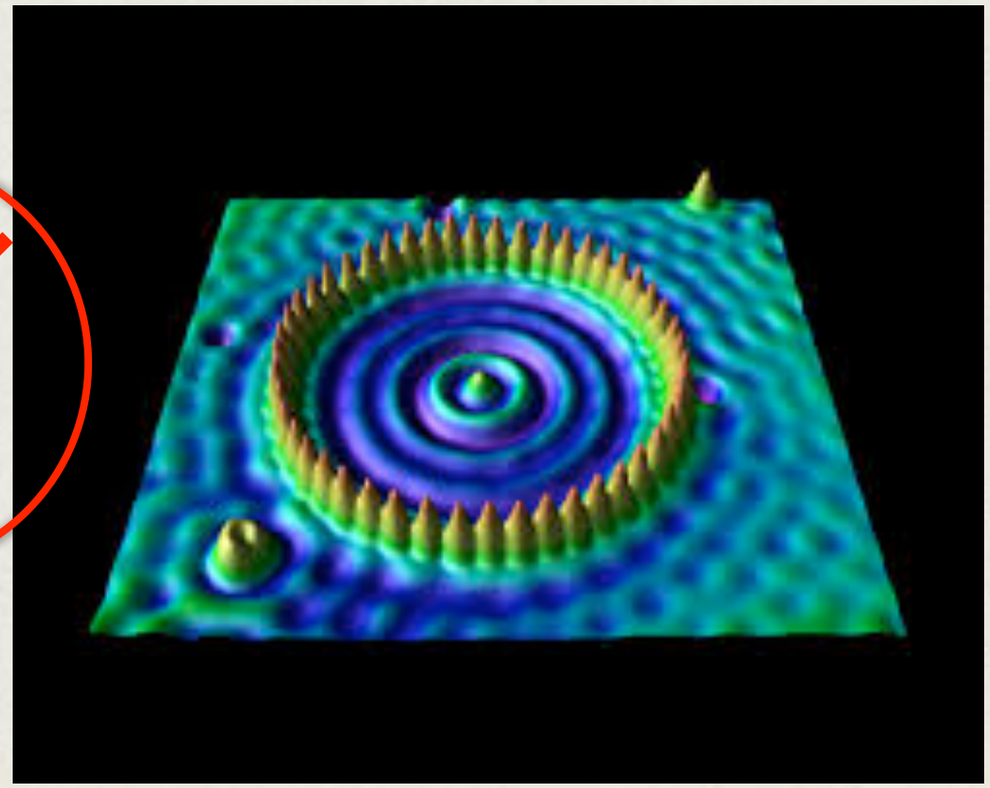
- Rows and columns indexed by N bit binary numbers with N_e 1's
- $|H_{ab}|$ equal to f(i,j,k,l) where a->b by turning off (i,j) and on (k,l)
- Sign[H_{ab}] depends on parity of electrons between (i,j,k,l)

Only N^4 non-zeros per row

Sparse and structure-full….

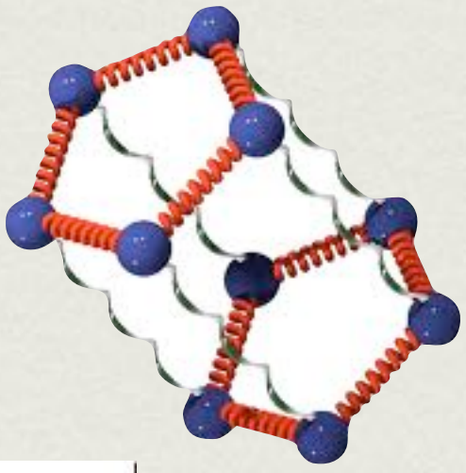




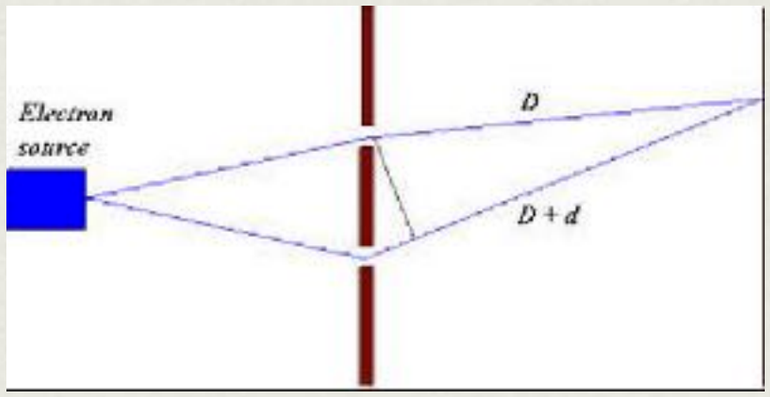


Q. Why can't classical computers simulate quantum system?
(i.e. what special about quantum mechanics)

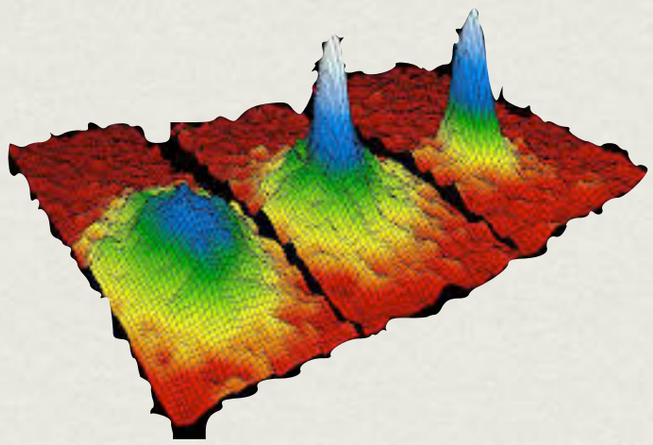
- Zero point motion and l_2 norm



- Interference



- Statistics



We are weighing classical computers against (small) quantum computers. What can classical computers do?

'Lore': Sign-free ground states

Use quantum Monte Carlo....

This lore relies on fast mixing times of Markov chains (for path integral Monte Carlo) or a well controlled population (diffusion Monte Carlo).

* 'known' to diverge exponentially for typical systems

*Energy 'straightforward'; sampling $|\Psi|^2$ less-so

* No evidence of long mixing times if you start in correct phase

Low entanglement ground states

Use tensor networks....

Questions about finding low-entanglement ansatz

Harder in molecules because tensor networks rely on locality (except for CGTNS*)

* Bauer, et al

Some philosophy …

The wave-functions you find in nature are often ‘simple’ and full of structure. It maybe shouldn’t surprise us, then, that approximating ground states of natural Hamiltonians shouldn’t be that “hard” for classical computers.

Evidence of Simplicity

- ☐ Energy ‘converges’: 1000 and 10^{10} similar.
- ☐ Probably not volume law
- ☐ Sign structure doesn’t alternate on short wave-lengths

- ☐ Constant depth quantum circuit
- ☐ Log depth quantum circuit
- ☐ Linear depth quantum circuit

Nature is mainly here

Even for sign-problem highly-entangled problems there are often classical algorithms which achieve a ‘good enough’ approximation.

Metric of ‘good enough’: chemical accuracy

1 milliHartree (out of 100 Hartree)

<u>To chemical accuracy:</u>

N=50 spin orbitals - Lancoz

N=70 spin orbitals - Tensor Networks

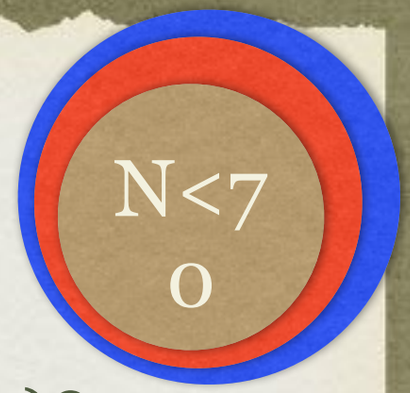
N>>100 spin orbitals - CCSD(T) on weakly correlated

Electrons ~ 30 - QMC Variants

ED: 1 site per year

Tensor Networks: ~10 site per year

Aside: Any QC algorithm ~30-50 qubits simulatable
38 qbits -> 10 minutes per step

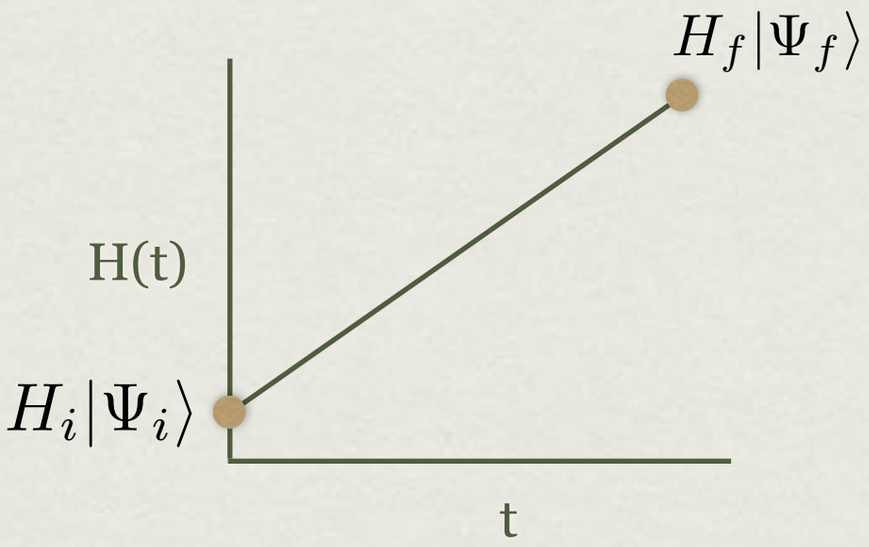


The quantum algorithm for getting ground state (energies)?

Two generic approaches

Adiabatic

- Start in Ψ_i as ground state of H_i
- $\exp[-itH(t)]$



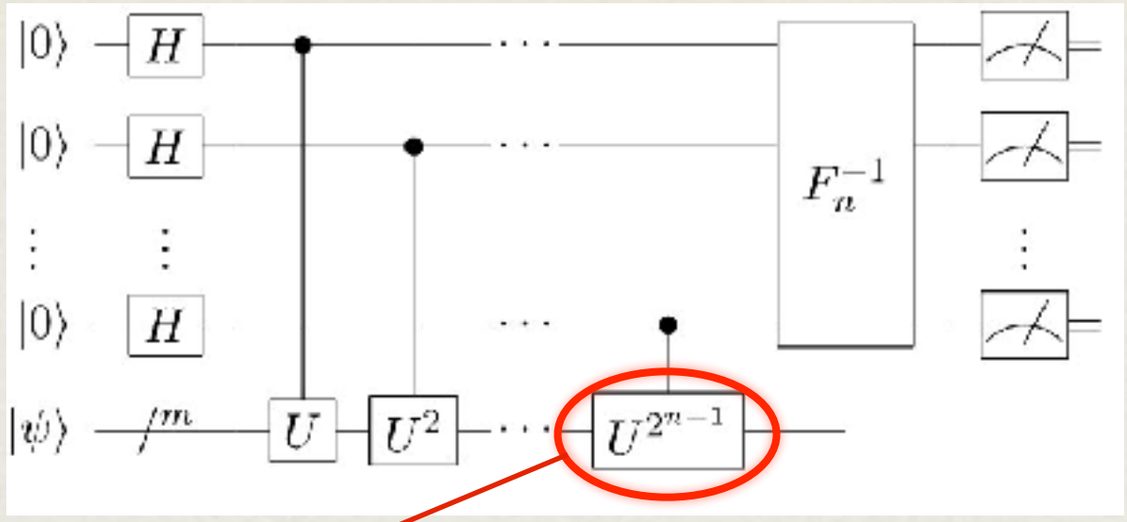
Phase Estimation

- Start close to ground state: $|\Psi_T\rangle = \sum_i \alpha_i |0\rangle|\Psi_i\rangle$
- Apply Phase Estimation: $\sum_i \alpha_i |E_i\rangle|\Psi_i\rangle$
- Measure E_i with probability α_i^2 getting Ψ_i

Let's just worry about this for the moment...

Quantum Phase Estimation

How quickly can this be done?



e^{-iTH} This is your computational bottleneck.

Algorithms

- Trotter Decomposition
- Sparse Hamiltonian Problem
  - Quantum Walks
  - Trotter

What T do we need?

Set by required accuracy: $T \approx 6000 E_h^{-1}$

Interesting note: What matters is absolute accuracy not relative accuracy.

Quantum Phase Estimation

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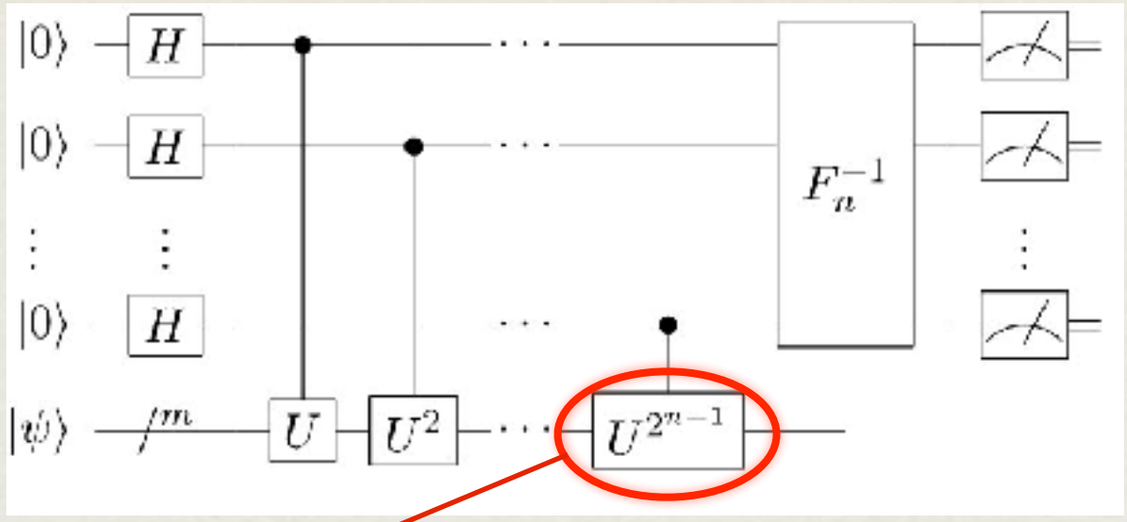

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Trotter

$$\exp[-itH]^{T/t}$$

$$\exp\left[-it\sum_{pqrs} V_{pqrs} c_p^\dagger c_q^\dagger c_r c_s\right]^{T/t}$$

$$\approx$$

$$\left(\prod_{pqrs} \exp\left[-itV_{pqrs} c_p^\dagger c_q^\dagger c_r c_s\right]\right)^{T/t}$$

# of trotter steps

Cost per term

How many terms?

Parallel Circuit	Global $\mathbf{R}_z$	$\mathbf{H}$, $\mathbf{Y}$, $\mathbf{Y}^\dagger$	CNOT	$\mathbf{CR}_z$	BSM	Total
H_{pp}	1			1		1
H_{pq}		8	2	4	4	18
H_{pqqp}			2	3		1+5
H_{pqqr}		4	8	4	4	24
H_{pqrs}		$8 \cdot 2$	$8 \cdot 2$	$8 \cdot 1$	$8 \cdot 2$	$8 \cdot 7$

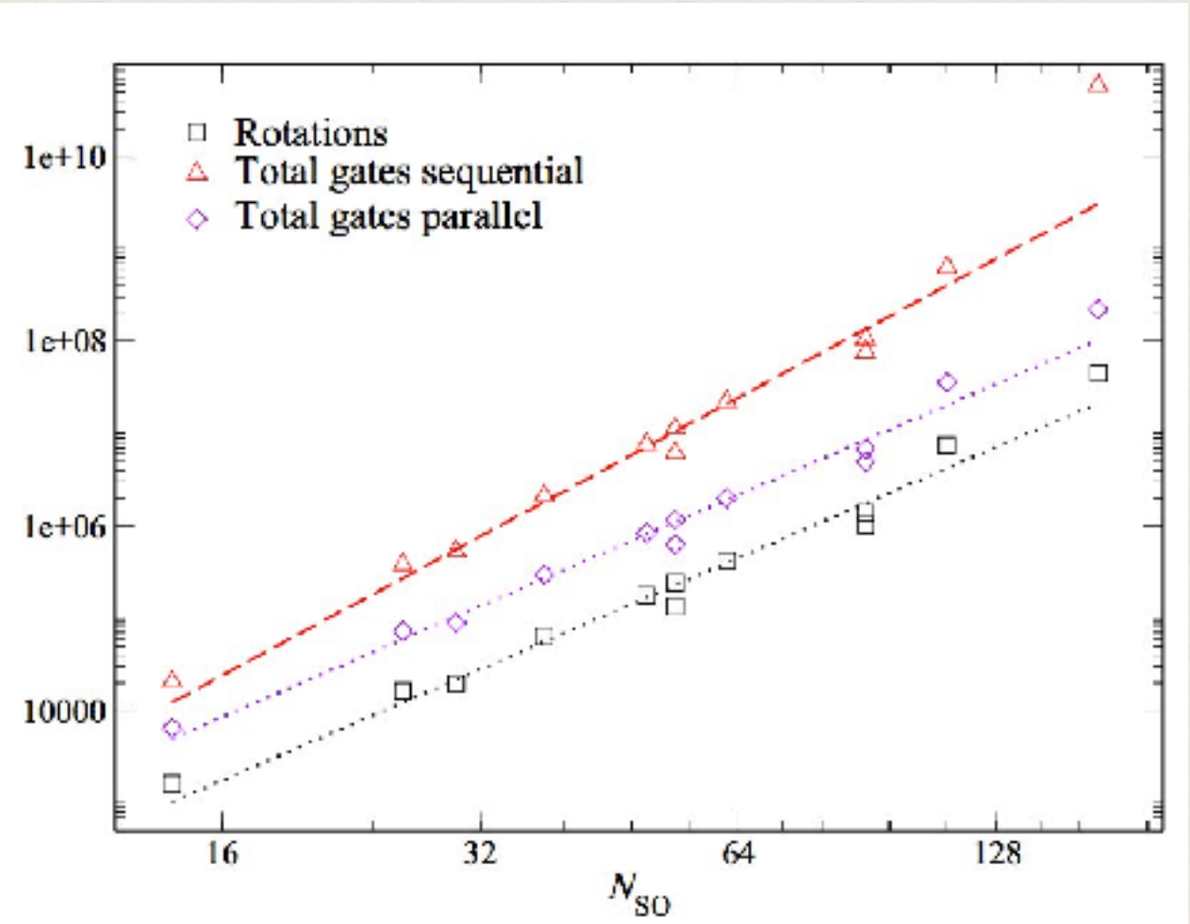
Computing number of gates: $O(\underline{N^4} \times \underline{N}) = O(N^5)$

terms in Hamiltonian

Jordan-Wigner strings for sign

Some of this back from parallelization

Matches empirically



Computing $1/\tau$

Theory: # trotter steps for fixed time (for fixed trace norm distance)

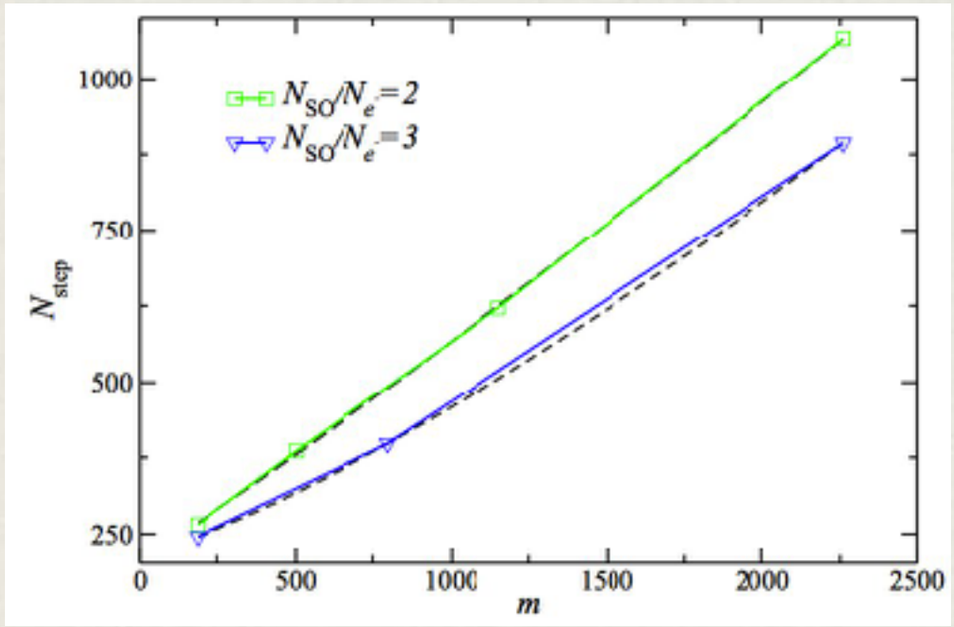
$O(\underline{m}^{1+1/\underline{2k}})$ m: terms in Hamiltonian | For k=1: $m^{3/2}$

k: trotter order

O(n) terms mutually commute. New theoretical bound:

For k=1: $Km^{1/2} \sim m^{3/4}m^{1/2} \sim m^{1.25}$

Empirically: # trotter steps for fixed time (for fixed energy error)



- Computed with imaginary molecules
- For k=1, $m^{1.08}$ - $m^{1.27}$

terms in trotter series $m \sim N^4$

Scaling: N^4- N^5

Putting it together …

(Gates per trotter step) x (Steps per fixed time) x (time)

N_g $1/\tau$ T

N^5 N^4 $6000 E_h^{-1}$

$$6000 N^9$$

Water (STO-3G): 10^{10} serial gates (441 x 441 matrix - 14 s.o.)
(by counting)

Fe_2S_2 (STO-3G): 10^{18} serial gates (112 s.o.)
(by extrapolation)

75 years of quantum Moore's law

Parallelization saves factor of 20

With 100 qubits, can never save more then factor of 100

In parallel: $6000 N^8$

What's the runtime?

	Logical Qubit time	Computation time
'Fast'	1 micro-second	3000 years
'Fantasy'	1 ns	3 years

Plus…no checkpointing!

This is (no matter how good hardware gets) unrealistic.

- Can we do better?
- Is their anything better already in the literature?

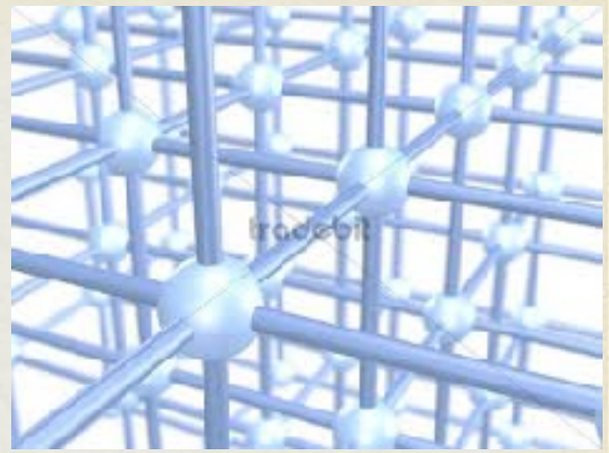
Localized orbitals

(Gates per trotter step)	x	(Steps per fixed time)	=	Total
	N_g	$1/\tau$		
quartic:	N^5	N^4		N^9
quadratic:	N^3	$N^{3/2}$		$N^{4.5}$

10,000 localized orbitals <---> 100 delocalized orbitals

Real Space

$$e^{-H} = e^{-K} e^{-V}$$



(Gates per trotter step)	x	(Steps per fixed time)	=	Total
	N_g	$1/\tau$		
quartic:	N^5	N^4		N^9
	N^2	2		N^2

1 million grid points <---> 100 delocalized orbitals

100 points per dimension

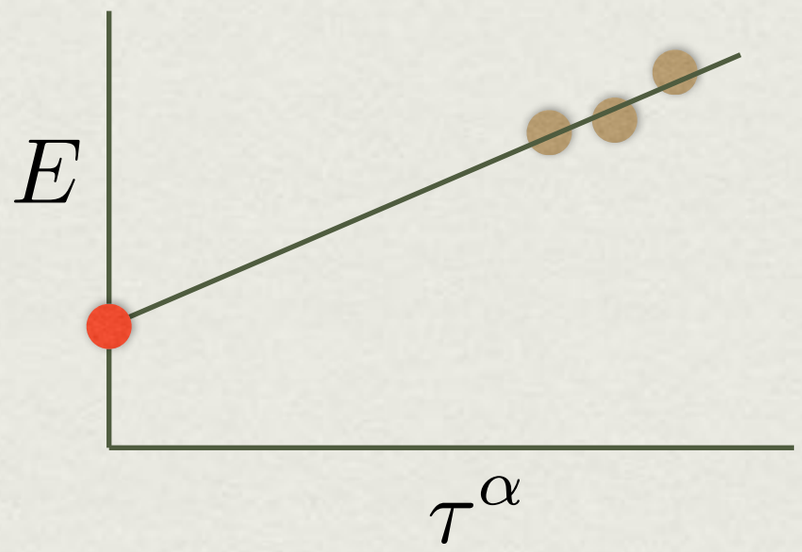
Other problems: Antisymmetrization, etc.

Other Approaches

Different breakup

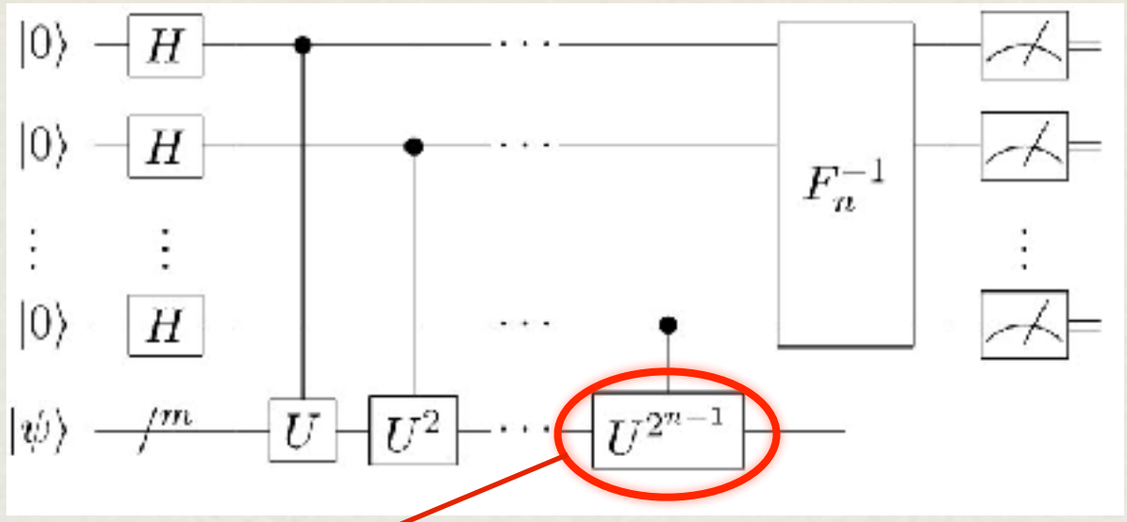
$$e^{-H} = e^{-h_1} e^{-h_2} e^{-h_3} \cdots e^{-h_n}$$

Time step extrapolation:



Quantum Phase Estimation

How quickly can this be done?



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  - Quantum Walks

What T do we need?

Set by required accuracy: $T \approx 6000 E_h^{-1}$

Interesting note: What matters is absolute accuracy not relative accuracy.

We also need to evaluate $1/\tau$ and number of gates.

Sparse Hamiltonian Problem

Given an oracle to elements of $H = \sum_{j=1}^{m} H_j$, compute $\exp[-iTH]$

d non-zeros per row

Oracle: $U_f|x,i\rangle|0\rangle = |\phi_{x,i}\rangle|y_i, H_{x,y_i}\rangle$

Quantum chemistry Hamiltonian: $d = N^4$

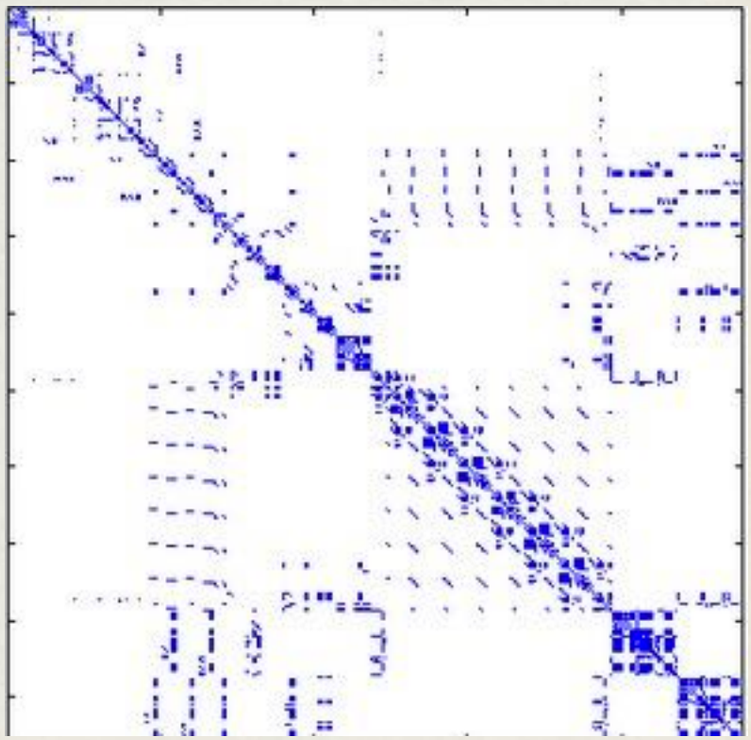
Two ‘current’ winners:

D. W. Berry, R. Cleve, and R. D. Somma, Preprint (2013), arXiv:1308.5424.

‘Trotter Approach’

D. W. Berry and A. M. Childs, Quantum Information & Computation **12**, 29 (2012).

‘Quantum Walks’



Trotter Steps*

$O(d^2 T \log^3(Td))$

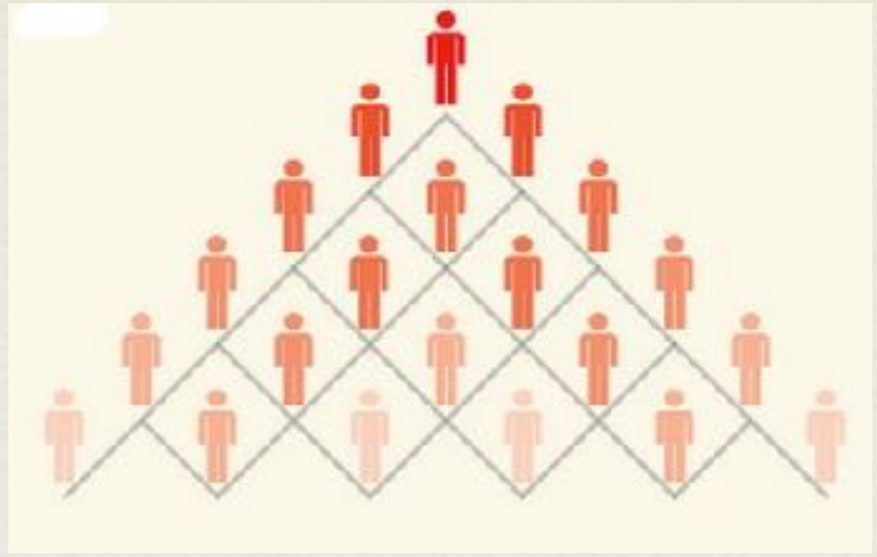
$O(N^8 T \log^3(TN^4))$ oracle queries.

Not much better then our current results.

Crossover $N \lesssim 100$

* D. W. Berry, R. Cleve, and R. D. Somma, Preprint (2013), arXiv:1308.5424.

Quantum Walks*



$$O(d^{2/3}((\log\log d)t||H||)^{4/3})$$

$$O(N^{8/3}((\log\log N^4)||H||)^{4/3})$$

$$||H|| \to O(N) \quad \text{(operator norm)}$$

$$O(N^{8/3}N^{4/3}((\log\log N^4))^{4/3}) = O(N^4) \quad \text{oracle queries}$$

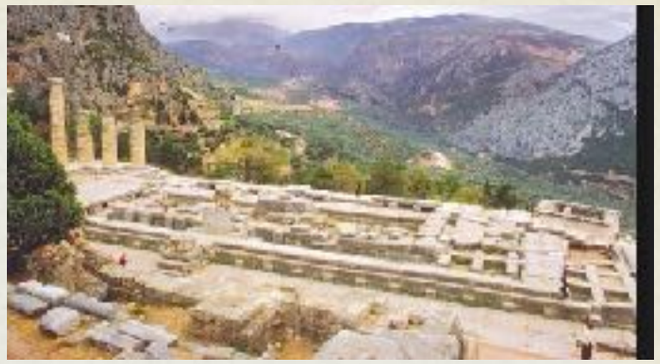
$$O(d\Lambda_{max}t)$$

$$O(N^4) \quad \text{oracle queries}$$

This looks quite promising.....

*Berry and Childs

until you think about the ‘oracle’...



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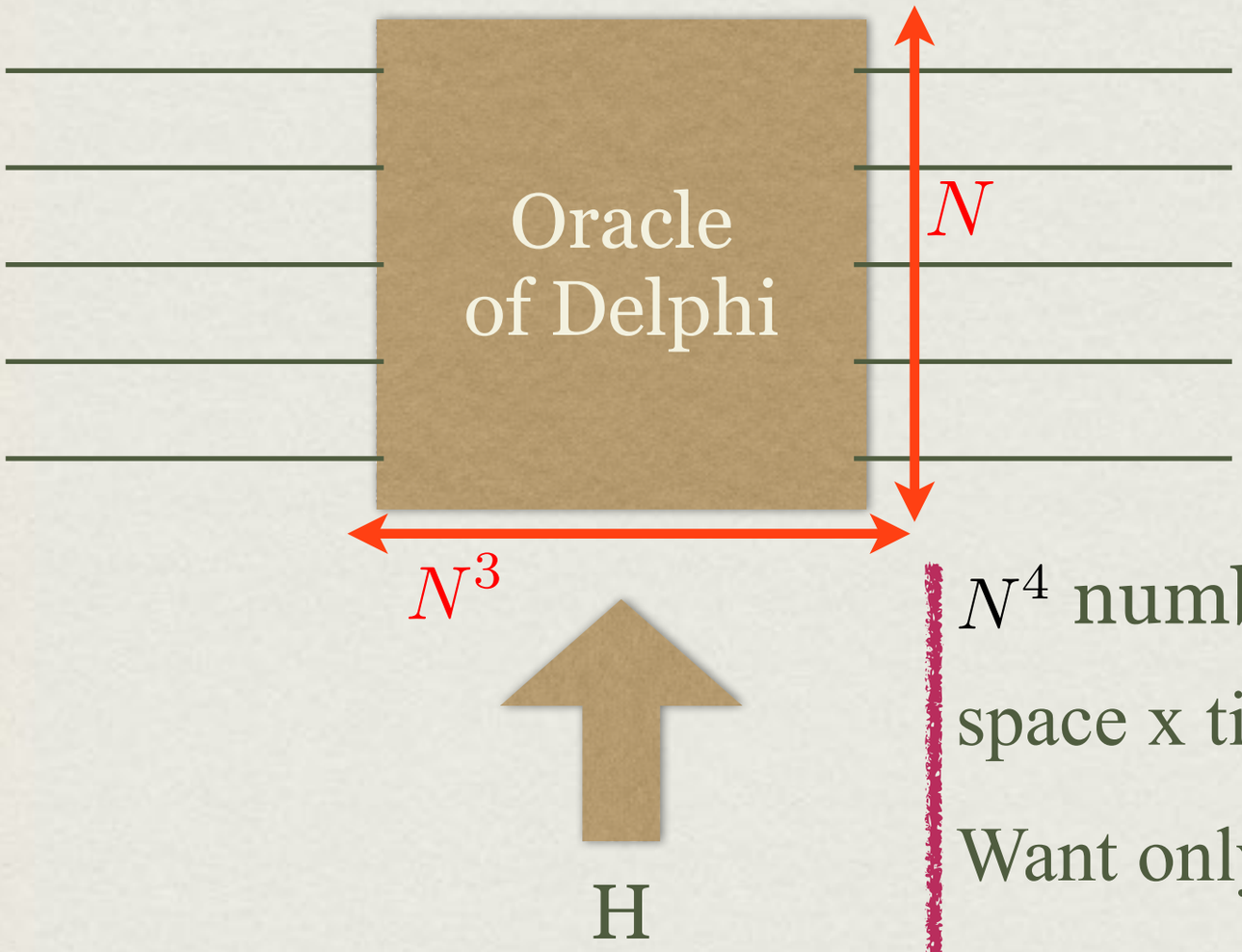


N^4 numbers in the box

space x time = N^4

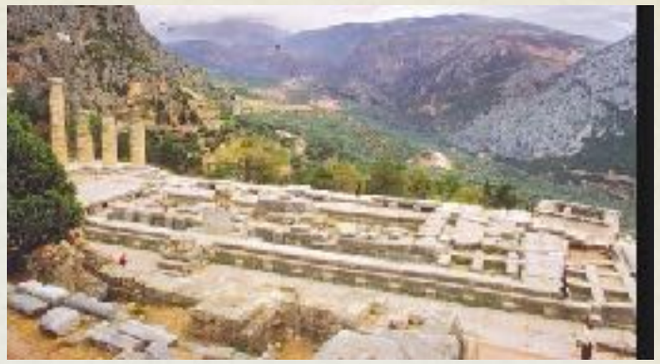
Want only N qubits

time: N^3 x N (Jordan-Wigner) = N^4

With quantum walks: N^8 time.

You can trade-off time for space here.

until you think about the 'oracle'...



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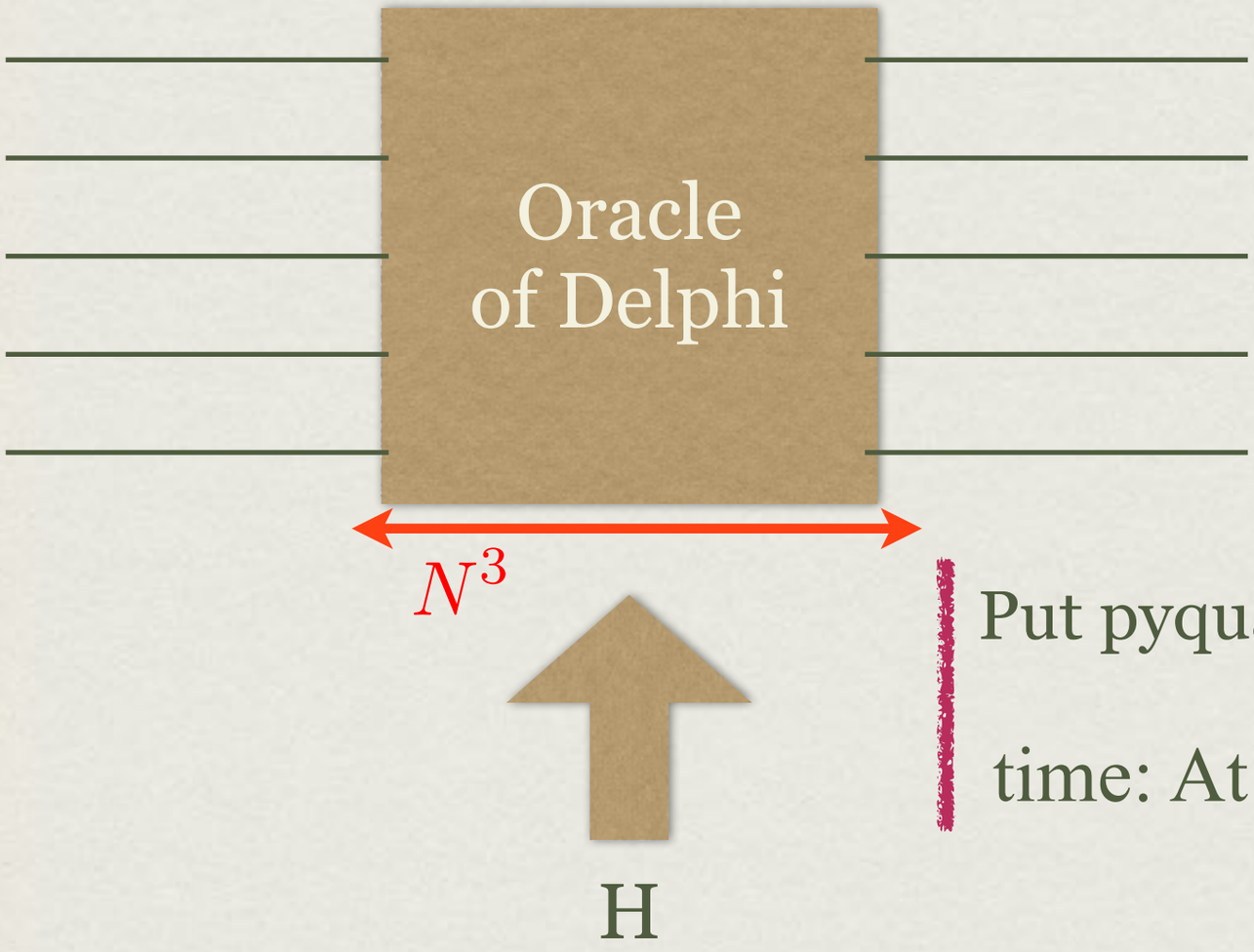


Put pyquante in the box

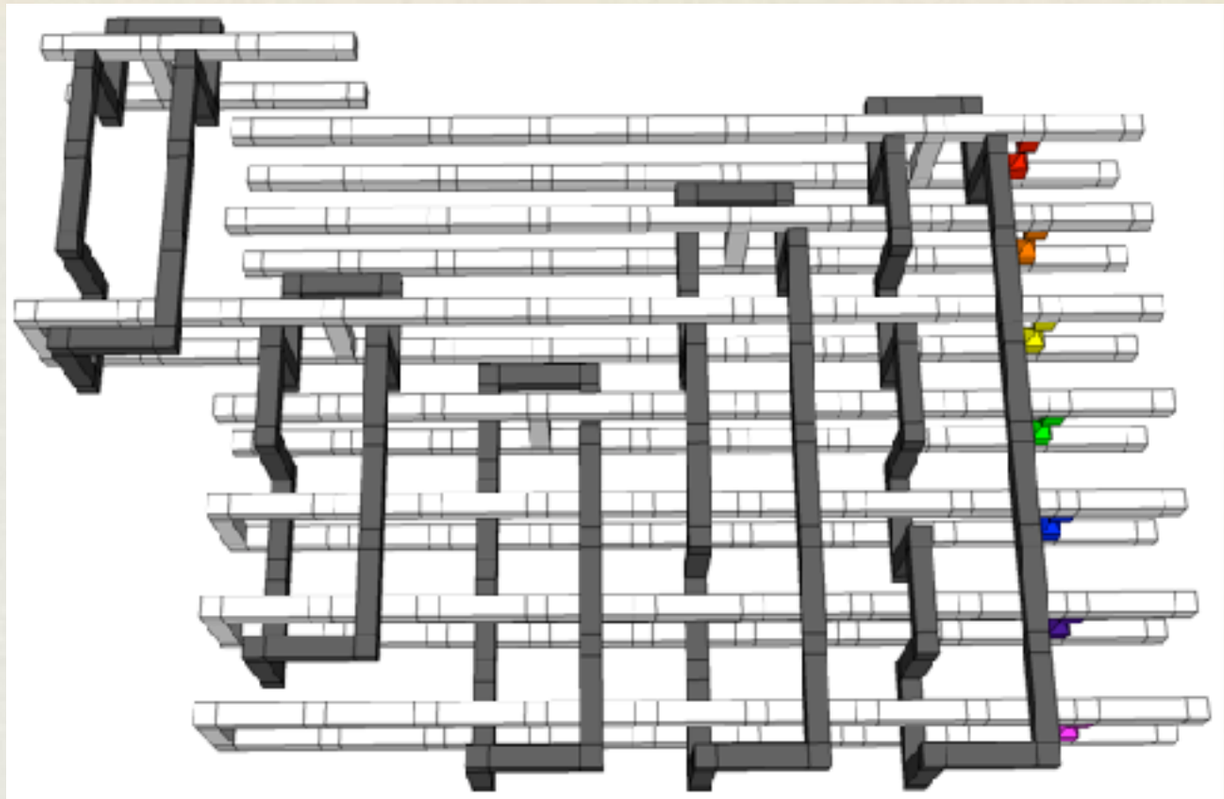
time: At least N^3 but probably more

With quantum walks: At least N^7 time.

What we've ignored....

- Error correction

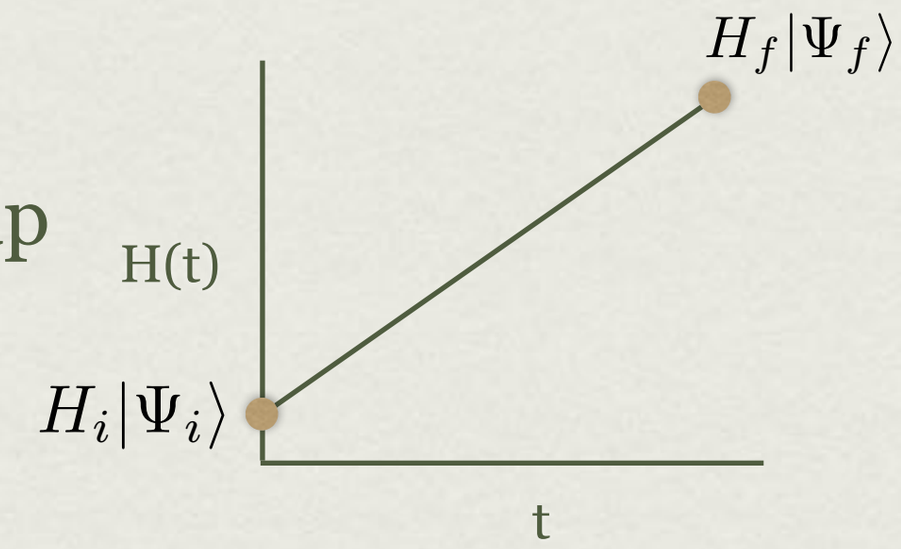
  ~ factor of 100



- Adiabatically evolving, measurements, ...

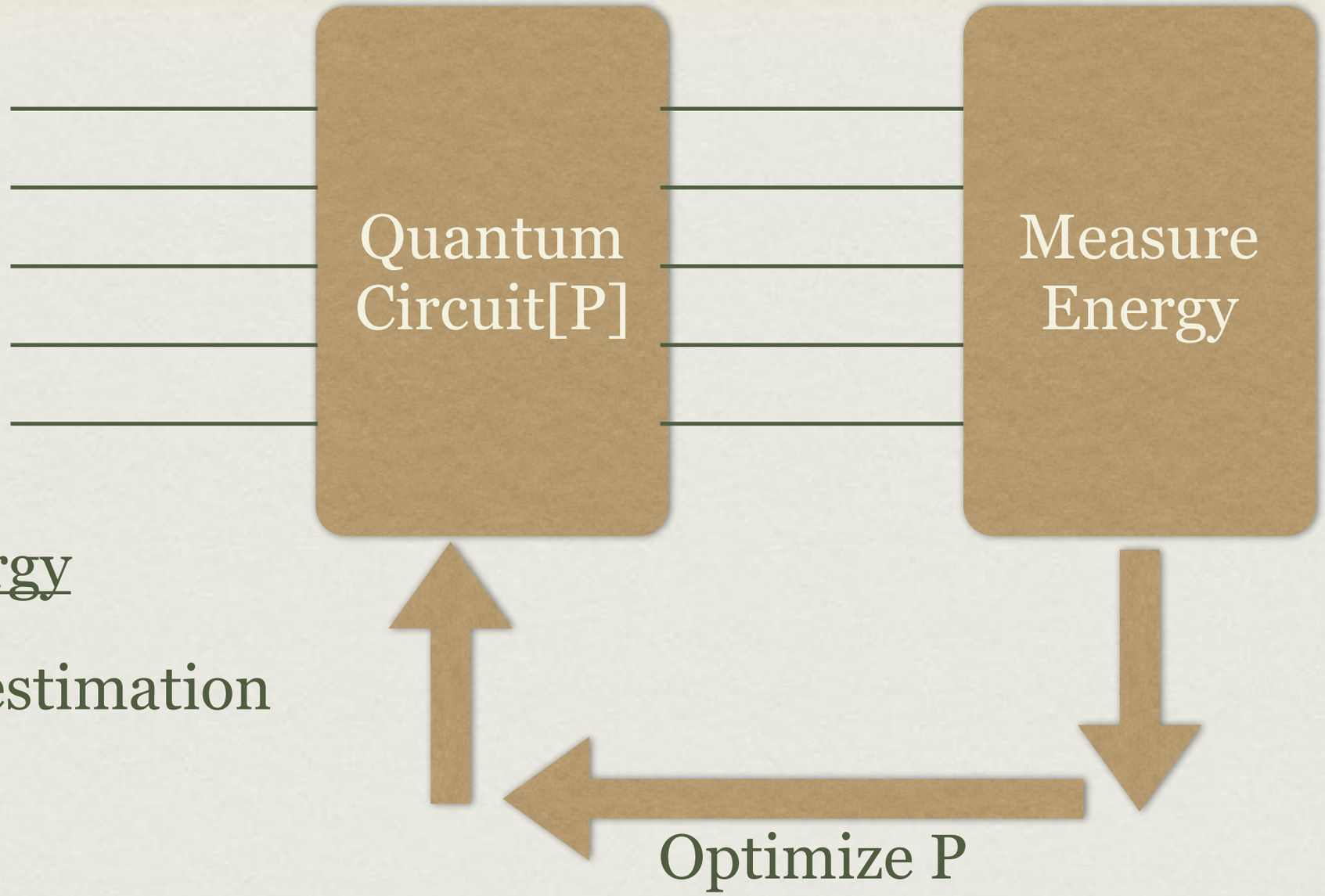
  Similar difficulties

  Speed depends on gap



Beyond Phase Estimation

Variational*



Measure energy

- ☐ Phase estimation
- ☐ Collapse

N^4 terms x N^2 scaling of Monte-Carlo Error = N^8

+

horrible non-linear optimization

* Apsuru Guzik

Adiabatic*

- $O(N^4)$ terms > 10^8
- $O(N^3)$ terms coupled to single qubit > 10^8
- 4 orders of magnitude range in accuracy
- Error correction?

* Aspuru Guzik

Summary

- Quantum mechanics in nature is full of structure …
  - classical computers are powerful …
    - and we don’t need arbitrarily low error…
      - This sets a high bar for quantum computation.

- Quantum chemistry on quantum computers scale around N^8
  - and it looks like we need 10^{18} gates to do something useful.

- Classical approximate algorithms scale better then exact quantum algorithms. When the approximation is good enough, go classical.